# Computational Optimization of Scramjets and Shock Tunnel Nozzles

by

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## **Statement of Originality**

The work presented in this thesis is, to the best of the author's knowledge and belief, original and the author's own, except as acknowledged in the text. The material contained in this thesis has not been submitted, either in whole or in part, for another degree at The University of Queensland or any other university.

Christopher S. Craddock

### Abstract

The design of supersonic flow paths for scramjet engines and high Mach number shock tunnel nozzles is complicated by high temperature flow effects and multidimensional inviscid/viscous flow interactions. Due to these complications, design in the past has been enabled by making flow modelling simplifications that detract from the accuracy of the flow analysis. A relatively new approach to designing aerodynamic bodies, which automates design and does not require as many simplifying assumptions to be effective, is the coupling of a computational flow solver to an optimization algorithm. In this study, a new three-dimensional space-marching computational flow solver is developed and coupled to a gradient-search optimization algorithm. This new design tool is then used for the design optimization of an axisymmetric scramjet flow path and two high Mach number shock tunnel nozzles.

The flow solver used in the design tool is an explicit, upwind, space-marching, finitevolume solver for integrating the three-dimensional parabolized Navier-Stokes equations. It is developed with an emphasis on simplicity and efficiency. Cross-stream fluxes are calculated using Toro's efficient upwind, linearized, approximate Riemann solver in flow regions of slowly varying data, and an Osher type solver in the remainder of the flow. Vigneron's technique of splitting the streamwise pressure gradient in subsonic regions is used to stabilise the flux calculations. A three-dimensional implementation of an algebraic turbulence model, a finite-rate chemistry model and a thermodynamic equilibrium model are also implemented within the solver. A range of test cases is performed to (1) validate and verify the phenomenological models implemented within the solver, thereby ensuring the simulation results used for design are credible, and (2) demonstrate the speed of the solver.

The first application of the new computational design tool is the design of a scramjet flow path, which is optimized for maximum axial thrust at a flight Mach number of 12. The optimization of a scramjet flow path has been examined previously, however, this study differs to others published in that the flow is modelled using a turbulence model and a finite-rate chemical reaction model which add to the fidelity of the simulations. The external shape of the scramjet vehicle is constrained early on in the design process, therefore, the design of the scramjet is restricted to the internal flow path. Because of this constraint, and the large internal surface area of the combustor and the high skin friction within the combustor, the net calculated force exerted on the scramjet for both the initial and optimized design is a drag force. The drag force of the initial design, however, is reduced by 60% through optimization.

The second application of the design tool is the wall contour of an axisymmetric Mach 7 shock tunnel nozzle, which is computationally optimized for minimum test core flow variation to a level of  $\pm 0.019^{\circ}$  for the flow angularity and  $\pm 0.26\%$  for the Pitot pressure. The design is verified by constructing a nozzle with the optimized wall contour and conducting experimental Pitot surveys of the nozzle exit flow. The measured standard deviation in core flow Pitot pressure is 1.6%. However, because there is a large amount of experimental noise, it is expected that the actual core flow uniformity may be better than indicated by the raw experimental data.

The last application of the computational design tool is a contoured Mach 7 square cross-section shock tunnel nozzle. This is a three-dimensional optimization problem that demonstrates the versatility of the design tool, since the effort required to implement the optimization algorithm is independent of the flow-field complexity and flow solver. Optimization results show that the variation in the test core flow properties could only be reduced to a Mach number variation of  $\pm 7\%$  and flow angle variation of  $\pm 1.2^{\circ}$ , for a short nozzle suitable for a shock tunnel. The magnitudes of the optimized nozzle exit flow deviations for the short nozzle and two other longer nozzles indicate that generating uniform flow becomes increasingly difficult as the length of square cross-section nozzles is reduced. Overall, the current research shows that coupling a flow solver to an optimization algorithm is an effective and insightful way of designing scramjets and shock tunnel nozzles.

## **List of Publications**

Craddock, C., "B-spline Surfaces for CFD Grid Generation," Department of Mechanical Engineering Report 1/95, The University of Queensland, Brisbane, Australia, January 1995.

Jacobs, P. and Craddock, C., "Simulation and Optimisation of Three-Dimensional Flows in Scramjet Ducts," *Twelfth International Symposium on Air Breathing Engines.*, edited by F. S. Billig, Melbourne, September 1995.

Craddock, C., "A Quasi-One-Dimensional Space-Marching Flow Solver with Finite Rate Chemical Effects," Department of Mechanical Engineering Report 7/96, The University of Queensland, Brisbane, Australia, June 1996.

Craddock, C. and Jacobs, P., "A Space-Marching Compressible Flow Solver with Chemistry and Optimization," Department of Mechanical Engineering Report 6/98, The University of Queensland, Brisbane, Australia, June 1998.

Craddock, C. S., Jacobs, P. A., and Gammie, R., "Operational Instructions for the Small Shock Tunnel at UQ," Department of Mechanical Engineering Report 8/98, University of Queensland, July 1998

Jacobs, P. A. and Craddock, C. S., "Simulation and Optimisation of Heated, Inviscid Flows in Scramjet Ducts," *Journal of Propulsion and Power*, Vol. 15, No. 1, 1999.

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## Nomenclature

A	: side of cell area, m <sup>2</sup> ;
	constant in Sutherland's viscosity formula, kg/(m.s.K <sup>0.5</sup> )
$A_j$	: constant in Arrhenius law for reaction $j$ , cgs units
a	: local speed of sound, m/s
В	: constant in Sutherland's viscosity formula, K
C	: mass concentration, mol/kg; flow characteristics
$C_p$	: coefficient of heat capacity (constant pressure), J/(kg.K)
$C_v$	: coefficient of heat capacity (constant volume), J/(kg.K)
$\operatorname{CFL}$	: Courant-Friedrichs-Lewy number
D	: van Driest damping term
d	: distance from wall used in turbulence model, m
$E^{o}$	: molar internal energy, J/mole
$\mathrm{E}_{j}$	: activation energy of reaction $j$ , J/mol
E	: total specific internal energy, J/kg
e	: specific internal energy, J/kg
$\mathbf{F}$	: algebraic vector of fluxes in conservation equations
$f_i$	: mass fraction of species <i>i</i>
$G^{o}$	: molar Gibbs free energy, J/mol
$H^o$	: molar enthalpy, J/mol
$(\Delta H_f^o)_{T_R}$	: formation enthalpy for a reference temperature $T_R$ , J/mol
h	: specific enthalpy, J/kg
$\hat{i},\hat{j},\hat{k}$	: unit vectors in Cartesian coordinates
K	: equilibrium constant
$k_B$	: Boltzmann's constant, $1.38066 \times 10^{-23}$ J/K
$k_f$	: forward reaction rate
$k_r$	: reverse reaction rate
k	: coefficient of thermal conductivity, W/(m.K)
L	: characteristic length across a cell, m
l	: integer difference in stoichiometric coefficients
М	: Mach number

M	: Molecular weight, g/mol
N	: number of exit plane computational cells within the nozzle core flow
$N_j$	: constant in Arrhenius law for reaction j
$N_R$	: number of reactions
$N_S$	: number of species
$\hat{n}$	: unit normal vector
$\overline{P}$	: position vector
p	: pressure, Pa
$p_{\mathrm{atm}}$	: standard atmospheric pressure, $101.3 \times 10^3$ Pa
Pr	: Prandtl number, $C_p \mu/k$
$\mathbf{Q}$	: algebraic vector of source terms in conservation equations
q	: viscous heat flux, J/(m <sup>2</sup> .s)
$R^o$	: universal gas constant, 8.31451 J/(mol.K)
$R_i$	: gas constant for species <i>i</i> , J/(kg.K)
$\tilde{R}$	: mixture gas constant, J/(kg.K)
Re	: Reynolds number
r	: radial coordinate, m
$S^o$	: molar entropy, J/(mol.K)
S	: control surface of the cell
dS	: cell-interface area, m <sup>2</sup>
T	: temperature, K
$T^*$	: reduced temperature
t	: time, s
$t_{\rm vib}$	: vibrational relaxation time, s
$t_{\rm fluid}$	: fluid dynamic characteristic time, s
$\hat{t}_1, \hat{t}_2$	: unit tangent vectors
$\Delta t$	: time step, s
U	: algebraic vector of conserved quantities
u	: velocity, m/s
V	: volume, m <sup>3</sup>
$X_i$	: mole fraction of species <i>i</i>
x, y, z	: Cartesian coordinates, m
$Z_i$	: chemical symbol of species i

 $\beta$ : compression parameter in the MUSCL interpolation/extrapolation; grid compression parameter : ratio of specific heats  $C_p/C_v$  $\gamma$  $\delta^*$ : boundary layer displacement thickness : characteristic energy, J  $\epsilon$ : Vigneron's coefficient ε θ : activation temperature, K : spatial accuracy constant for MUSCL interpolation/extrapolation  $\kappa$ : second coefficient of viscosity, Pa.s λ : shear stress, Pa τ : coefficient of viscosity, Pa.s; equivalent molecular weight, g/mol  $\mu$ : density, kg/m<sup>3</sup> ρ : collision diameter, Å  $\sigma$ Φ : safety factor for Vigneron's pressure splitting : term in Wilke's viscosity law; generalized flow variable  $\phi$ ψ : half angle for axisymmetric cells, rad : axisymmetric cell volume per unit radian, m<sup>3</sup>/rad Ω  $\Omega^{(2,2)}$ : elastic collision integral : axial flow vorticity,  $s^{-1}$ ω : production rate of species per unit volume, kg/(s.m<sup>3</sup>) ŵ  $\xi, \eta, \zeta$ : normalized coordinates

#### Superscripts

 $\alpha$ 

T	: transpose
0	: molar quantity
/	: reactant
//	: product
n	: time level
u	: pertaining to the up-stream vertex slice
	: time differential
*	: nozzle throat condition

#### Subscripts

$\infty$	: free-stream value
A, B, C, D	: vertex labels
ix, iy, iz	: cell-centre indices
$ix \pm \frac{1}{2}$	: vertical, streamwise interface
$iz \pm \frac{1}{2}$	: vertical, cross-stream interface
$iy \pm \frac{1}{2}$	: horizontal, cross-stream interface
i	: inviscid contribution to fluxes
i	: species number
j	: reaction number
lam	: laminar
L	: left state
MIN	: minimum value
N, S, E, W	: North, South, East, West interface or boundary
n	: normal to interface
R	: reference; right state
s	: stagnation condition
t	: tangent to interface
turb	: turbulent
v	: viscous contribution to fluxes
wall	: wall value

### Introduction

In the 1950s and 1960s, the threat of the "cold war" and the race for the moon motivated pioneering research in the area of hypersonics. Later, in the 1980's, projects such as the American National Aerospace Plane (NASP) built on this pioneering research and looked at the feasibility of a single-stage-to-orbit reusable flight vehicle. Research in this field is still being undertaken today with projects such as NASA's Hyper-X hypersonic experimental research vehicle [67, 230], which focus on the challenges of developing single-stage-to-orbit technologies, reducing launch costs and ultimately, increasing access to space.

Essential to the development of single-stage-to-orbit flight vehicles has been the propulsion system and one of the proposed systems that shows great promise is the supersonic combustion ramjet or "scramjet". A scramjet is an air-breathing engine that operates at hypersonic flight speeds (above Mach 6) and maintains supersonic flow conditions throughout its operating cycle. The inception of the scramjet can be traced back to 1958 when Weber & Mackay [233] investigated the possibility of performing combustion within a supersonic flow in order to overcome the flight speed limitations of the ramjet. At hypersonic flight speeds, the total pressure losses incurred through the normal shock that decelerates the flow in the ramjet makes the use of the engine impractical. Also, combustion becomes inefficient because the high post-shock temperatures prevent energy releasing combustion products from forming. However, if the inlet flow is processed by oblique shocks and combustion takes place in a supersonic flow, the efficiency of the engine is increased to practical levels. This theory was extensively tested and developed in the 1960's by Ferri [63, 64] and Swithenbank [215] who both made important contributions in the area. Since then, research into scramjet propulsion has continued but, as of yet, only limited success has been achieved in building a functional scramjet engine that is capable of supersonic combustion in flight [184].

Part of the reason for the slow pace of scramjet research is the complex nature of the high temperature flows that are present within the scramjet engine. Modelling these flows accurately and making informed design decisions based on analysis is a formidable task. Another reason is the difficulty of generating high quality test flows at high Mach numbers

in ground-based wind tunnels. Many of the present facilities used for scramjet research produce high Mach number flows of low quality in terms of the flow uniformity. The quality is poor because the nozzles that are used to expand the test flow to high Mach numbers are generally designed using assumptions that become invalid at high Mach numbers.

The aim of this thesis is to address these two design issues related to scramjet research by developing and applying a computational design tool for supersonic flow ducts. The tool, which couples a parabolized Navier Stokes flow solver with an optimization algorithm, is applied specifically to: (i) the design of a Mach 12 axisymmetric scramjet engine flow path; and (ii) the design of high quality Mach 7 hypersonic nozzle contours for a reflected shock tunnel. In this introductory chapter, a background for both scramjet and shock tunnel nozzle design is given along with the motivation for using computational methods to address these design problems. A strategy for applying computational methods to hypersonic design is then discussed followed by a review of the contents of the chapters that follow.

### **1.1 The Scramjet Engine**

The principles of scramjet operation have not changed appreciably since the pioneering work of Weber & Mackay [233] in the 1950's, and Ferri [63, 64] and Swithenbank [215] in the 1960's. A large part of the research effort since then has been focused on high temperature flow mechanisms that hinder the engine concept from being practically applied to flight vehicles such as manned hypersonic aircraft, transatmospheric accelerators, and missiles. Some areas of interest have been combustion and fuel mixing efficiency, thermal load and skin friction reduction, and engine starting. The Department of Mechanical Engineering at The University of Queensland has undertaken research in these areas since the early 1980's with the goal of manufacturing and flight-testing a scramjet-powered vehicle. To date, this goal has proved elusive.

One of the scramjet concepts that has been studied within the department is an axisymmetric scramjet to be used as a second stage for a small launch vehicle as shown in Fig. 1.1 [112]. Part of the motivation for pursuing this concept is the scaling argument put forward by Stalker [209]. His study suggested that a small launch vehicle, with a scramjet-powered second stage and the capability of placing a 1000kg payload into low earth orbit, can be operated competitively against traditional, all-rocket launch vehicles. The design concept is based on the accelerator vehicle studied by NASA [43], which has a conical forebody and a set of scramjet modules surrounding the centre body. Separate scramjet modules facilitate differential throttling, which aids in control of the vehicle. Each module is highly integrated with the forebody and afterbody of the stage to reduce total vehicle drag at hypersonic speeds, as well as to reduce total weight. High integration



Figure 1.1: A launch vehicle concept that uses a scramjet for second stage propulsion.

of the engine and vehicle are common to most scramjet concepts [161] and high-speed vehicles, which have inherently narrow performance margins [140].

The flow processes of the scramjet engine module can be described with reference to Fig. 1.2. Free-stream hypersonic air entering the scramjet is first compressed by a series



Figure 1.2: Schematic of a body integrated scramjet module.

of oblique shocks emanating from the conical forebody, the inlet and the cowl. These shocks typically raise the temperature of the gas to at least 1000 K, and to a pressure on the order of 100 kPa (an atmosphere). Fuel is then injected into the hot, compressed supersonic air stream at the start of the combustor. Currently, hydrogen appears to be the most suitable fuel for scramjet combustion because of its high energy release per unit mass, high reactivity and its cooling capacity [101]. It does, however, require a larger containment volume compared to other candidate fuels.

Once injected, the fuel undergoes turbulent mixing with the air and "auto-ignites" due to the high temperature of the shock-compressed air. The fuel is mixed and burned as it travels the length of the combustor. The high enthalpy products created by combustion, together with the remaining unburnt air and fuel, are expanded by the vehicle afterbody thrust surface and cowl to a velocity and pressure slightly greater than the free-stream. The net thrust developed by the scramjet is the difference between the thrust generated by the expansion of the exhaust gases at the aft section of the engine, and the total drag on the engine. Both these opposing forces are of similar magnitude. As a result, there is a fine balance between an engine design that produces positive thrust and one that doesn't.

The thermodynamic cycle of a scramjet engine is essentially an open Brayton cycle where gas compression and expansion processes are used to develop thrust. The ideal performance of the engine is governed by the reversible Brayton cycle where fluid flowing through the device undergoes isentropic compression and expansion, and combustion occurs completely with no loss of total pressure. In reality, however, scramjet performance is far from ideal due to the many loss mechanisms and inefficiencies present in the flow, which ultimately result in a reduction of useful thrust. Three thrust loss mechanisms that are present through the entire scramjet engine are wall friction, heat removal, and total pressure loss due to shock waves. Other thrust losses that are associated with the combustor are fuel injection and mixing losses, quenching of combustion reactions, and incomplete combustion. The minimisation of these losses is not a simple matter since they are coupled to each other through their effects on the flow conditions within the scramjet.

Due to the complex interactions of loss mechanisms within the scramjet, designers have traditionally relied on simplified performance analyses and experimental testing to carry out applied research [215, 27]. Performance analyses usually take the form of parametric studies using efficient quasi-one-dimensional codes coupled with high temperature gas models [233, 119, 175]. These studies are useful for providing an insight into the relationship between engine performance and high temperature flow mechanisms, performance limits of an actual engine, and identifying guidelines for design [100]. However, they generally do not provide results of quantitative significance because they do not include all of the important multidimensional flow interactions that are present in the actual flow within a scramjet [119]. Quantitative results are obtained through experimental testing of scaled models in hypersonic wind tunnels where effects such as viscous drag and heating, turbulent mixing, and finite-rate chemical kinetics can be simulated. These results can then be analysed and used to extend the designers understanding of the flow processes within the engine and ultimately improve the design. Presently, however, ground-testing facilities are only capable of simulating flows within a narrow range of flight Mach numbers for the trajectory of an actual scramjet [6]. Despite this shortcoming, experimental testing has been one of the only practical ways of undertaking scramjet design up until recent times.

Computational methods have now reached a level of maturity where flow solvers can be used to perform the flow tests that were otherwise only achievable in ground-based facilities. Further, computers can be used as tools to analyse and design hypersonic vehicles at high Mach numbers where ground-based facilities cannot match the flight enthalpies, and they can extend results from ground-based facilities to full-scale flight conditions [124]. However, flow solvers are only as good as the phenomenological models that are built into the solver. Hence, there will be a continuing need for experimental facilities to validate the models used in flow solvers [75]. Having validated a flow solver, it can be used to reduce design cycle time and provide useful insights into scramjet flow mechanisms that are not always possible with experimental methods. Moreover, flow solvers can be coupled to optimization algorithms to automate design and identify flow mechanisms that improve or degrade the performance of scramjet engines.

### **1.2 Hypersonic Wind Tunnel Nozzles**

Ground-based wind tunnels have been used for the research and design of flight vehicles for the last 30 to 40 years. They provide a means of determining forces and pitching moments on scale models of flight vehicles in test flows that exhibit similar thermochemical flow characteristics to those experienced by full scale flight vehicles. In recent times, they have also been used to provide benchmark data for the calibration of CFD<sup>1</sup> flow solvers [77, 132, 126]. For both tasks, a uniform, hypersonic flow is required in the test section.

Due to the high enthalpy and high density of the flow through a scramjet in flight, the types of ground-based wind tunnels that can be used to simulate the high temperature effects in scramjet flow are not widely available. Compared with a rocket-based launch vehicle, the scramjet trajectory needs to be low and through a relatively dense part of the atmosphere because it requires atmospheric air to burn the fuel (see Fig. 1.3).

Ground-based wind tunnel facilities can be classed as either continuous flow, intermittent flow or pulse-type facilities. Continuous and intermittent flow wind tunnels that match only scramjet flight Mach numbers are plentiful since hypersonic test flows can be generated by steadily expanding a high pressure reservoir of gas at ambient temperature through a nozzle with an appropriately large expansion ratio. However, the temperature and, subsequently, the enthalpy of the test gas are low since the stagnation temperature is approximately room temperature. Facilities that use supply gas reservoirs at room temperature are typically limited to Mach numbers of approximately 4 because of problems with liquification of the expanding test gas. If high pressure gas at ambient temperature is expanded through a high Mach number nozzle, the temperature of the expanded gas can fall below the boiling point of the gas causing molecules to liquefy. This problem can be avoided by using gases such as helium [31] (an example is the 22 Inch Mach 20 helium blow-down tunnel at the NASA Langley research centre [150]), however, the hypersonic

<sup>&</sup>lt;sup>1</sup>Throughout this thesis, CFD refers to computational fluid dynamics using a digital computer



**Figure 1.3:** Typical ascent trajectory for a scramjet powered flight vehicle placing a payload into low earth orbit compared to the shuttle trajectory. The dashed lines show contours of dynamic pressure,  $q = \frac{1}{2}\rho_{\infty}u_{\infty}^2$  (adapted from Billig [27]).

test flows produced do not match the enthalpy and thermochemical characteristics of the flow in hypersonic flight through the atmosphere.

The problem of liquification can also be avoided by raising the enthalpy of the gas through heating prior to expansion. However, the large amount of energy required to heat the gas for high Mach number flows with matched flight enthalpies, and the problems with the containment of the gas supply, limits the use of this technique to the order of minutes or seconds. Various methods are used to heat the gas including passing the gas through a bed of heated pebbles, passing the gas through an electric arc, and heating through combustion then adding oxidant to make up the gas composition prior to combustion (vitiation).

Presently, the most effective and widely used class of ground-based wind tunnel facility that is capable of reproducing most of the flow conditions experienced by a scramjet in its flight trajectory is a pulse facility (i.e., shock tubes/tunnels and expansion tubes/tunnels). Pulse facilities use shocks and unsteady expansions to raise the enthalpy of a slug of gas, which is then expanded through a nozzle or accelerated into a test section at hypersonic speeds [205]. Large enthalpies that match re-entry, orbital and super-orbital flight speeds are achievable with pulse facilities, and the test gas can be made to exhibit the high temperature thermochemical effects experienced in high speed flight. However, the nature of the unsteady shock waves and expansions in these facilities limits the test time to the order of milli-seconds for test flow velocities less than approximately 4 km/s

and micro-seconds for test flow velocities greater than approximately 10 km/s.

One of the types of pulse facilities that generate test flows on the order of milli-seconds are reflected shock tunnels. Within a reflected shock tunnel, a high temperature slug of stagnated test gas is generated via an incident and a reflected shock. The incident shock is generated by exposing the test gas to a high pressure reservoir of "driver" gas through the rupture of a metal diaphragm at the upstream end of the shock tube. Various methods have been used to generate the high pressure driver gas that ruptures the diaphragm, including compressed air reservoirs, free piston compressors [204] and detonation waves [19]. The high temperature stagnated gas is then expanded through a nozzle to hypersonic conditions in the test section.

As a result of the high construction and running costs of reflected shock tunnels, there are few in service around the world at the present time compared to other types of hypersonic test facilities. Some of the well known reflected shock tunnels around the world are the Calspan shock tunnel (now known as Veridian), the Ames research centre shock tunnel, the T4 tunnel at The University of Queensland, the T5 shock tunnel at The California Institute of Technology, and the HEG shock tunnel at DLR Göttingen (see Anderson *et. al* [6] for a comparative performance review). All of these tunnels use a free piston to compress the driver gas.

The T4 free piston reflected shock tunnel at The University of Queensland [207] has several contoured axisymmetric nozzles that can be used to expand the shock heated test gas to the required Mach number in the test section. The current range of nozzles are Mach 4, 5, 8 and 10. The flow issuing from these nozzles is commonly used in a "direct connect" mode for testing scramjet combustors where the flow travels directly into the combustor. The process of compressing the flow through an inlet on the vehicle is not directly modelled. Therefore, the flow entering the combustor is nominally parallel and free of waves.

The design of all of the current T4 hypersonic axisymmetric nozzles was based on the classical method proposed by Prandtl & Buseman [11] in 1929. The method uses the method of characteristics (MOC) in an inverse design mode to determine an inviscid nozzle wall contour that produces the desired uniform exit flow. The contour is then corrected with a displacement thickness obtained from a boundary-layer (BL) calculation to account for the boundary layer that develops along the nozzle wall. The underlying assumption behind this method is that the boundary layer flow and core flow are uncoupled.

In low Mach number nozzles, where boundary layers are thin, the location where the flow characteristics reflect is closely approximated by the inviscid contour as assumed by the MOC/BL technique. However, for thick boundary layers, as developed in high Mach number nozzles, the flow characteristics effectively reflect between the wall and the

inviscid contour [36] such that the actual characteristic lags the design characteristic as shown in Fig. 1.4. Hypersonic nozzles designed for Mach numbers of 7 to 8 begin to



**Figure 1.4:** Lagging of actual characteristic from MOC/BL design characteristic due to a thick boundary layer on a nozzle wall

show this effect where turbulent boundary layers grow to a large percentage of the exit radius [25]. As a direct consequence of the miscalculation of characteristic reflection, complete cancellation of expansion waves is no longer achieved and the flow quality of the nozzle deteriorates.

The effect of the characteristic reflection miscalculation can be demonstrated by a comparison of Pitot surveys for the various T4 shock tunnel nozzles. The Mach 4 nozzle, which was designed using the MOC/BL method, has been shown to produce good quality test flow over a range of enthalpies (variation in core flow Pitot pressure across the exit plane  $\pm 5\%$ ) [104]. However, the higher Mach number nozzles show significant centre line disturbances within the test core (the Mach 10 nozzle has a variation in Pitot pressure of up to  $\pm 25\%$  for low stagnation pressures) [114, 115]. Figure 1.5 shows a typical Pitot profile of the flow issuing from the Mach 8 and Mach 10 nozzle for the T4 free piston shock tunnel at The University of Queensland [116, 115].



**Figure 1.5:** Normalised Pitot surveys of the T4 Shock Tunnel Mach 8 and Mach 10 nozzles. Error bars indicate standard deviation of signal noise over the steady test time.

Centre line disturbances in the nozzle exit flow were also shown to occur in all of the original axisymmetric contoured nozzles at the Langley Research Center Hypersonic Facilities Complex designed during the 1950's and 1960's [152, 77]. These nozzles were also designed using MOC/BL. Variations in the test flow Pitot pressure in excess of 30% were reported for the Mach 17 nozzle of the Langley 20 Inch nitrogen tunnel [153, 150]. Despite the non-uniformities in the nozzle exit flow of the Langley wind tunnels and the T4 shock tunnel, the nozzles have provided test flows of adequate quality to explore many of the basic design issues associated with scramjet engines and hypersonic flight in general. However, the resurgence of interest in hypersonics, and the need to obtain high quality flow data for CFD code validation, has provided the motivation for improving the flow quality afforded by these nozzles.

A relatively new nozzle design method that correctly models the interaction between the core flow and the boundary layer in high Mach number nozzles where the boundary layer becomes thick, involves coupling a computational flow solver and an optimization algorithm [125, 118, 222]. Computational flow solvers based on the Navier-Stokes equations can be used to calculate accurate flow solutions for a given nozzle design. The flow solution and nozzle contour can then be passed to an optimization algorithm, which perturbs the contour iteratively until the desired exit flow is achieved. The accuracy of the design method is limited only by the accuracy of the flow solver used to perform the flow-field calculations. Also, the design method is not limited to axisymmetric nozzles since it can be used for designing three-dimensional square cross-section nozzles by simply employing a three-dimensional flow solver. Designing three-dimensional nozzles with this method is computationally intensive and has only become practical in recent times because of advances in computer technology. The design calculations for a square cross-section nozzle shown later in this thesis typically required 75 hours to complete using one R10000 processor of The University of Queensland's SGI super-computer, and would have required over a month on a similar machine some years ago (based on the performance of the SGI R6000 processor released at the beginning of the 1990's).

#### **1.3 Design optimization using CFD Flow Solvers**

Having identified the advantages of using computational design optimization in the areas of scramjet design and high Mach number wind-tunnel nozzle design in the previous two sections, the method of computational design optimization can now be addressed. Design optimization using CFD flow solvers is an inverse design method where the desired flow characteristics or forces associated with an aerodynamic body are specified, and an attempt is made to find the shape that will produce the required flow characteristics or forces. Using a design tool based on a CFD flow solver and an optimization algorithm is a relatively new approach to aerodynamic design that seems to be superseding the use of many classical methods for problems involving complex non-linear flow phenomena [97]. Decades of improvements to computational techniques and models, together with

the rapid advancement in computer technology, has resulted in CFD flow solvers that are fast and capable of accurately modelling inviscid-viscous interactions with high temperature thermochemical effects. Computational design tools based on these flow solvers and iterative optimization algorithms are now practical alternatives to design through pure experimental research and classical analysis techniques, such as the method of characteristics.

The method of coupling flow solvers to optimization algorithms and applying them to aerodynamic design problems has not changed appreciably since the inception of the idea. One of the first studies that used the method for the design of nozzles and aerofoils was conducted by Huddleston [97]. Huddleston's optimization method essentially consisted of modelling an aerodynamic surface with a parametric curve and manipulating it in an iterative process. The surface manipulation was based on a performance function that quantified some undesirable quality of the flow around or through the body. For every prospective surface design, a flow solution was computed using a either a Navier-Stokes or Euler flow solver. Then the performance function, otherwise known as the objective function, was evaluated using data extracted from the flow solution. The objective function evaluation was then used by an optimization algorithm to determine new values of the design variables, which defined the aerodynamic surface. The iterative process continued until the flow produced by the body or the forces exerted by the flow on the body met the design requirements. The optimization process is illustrated in Fig. 1.6.



Figure 1.6: Design optimization using a CFD flow solver.

An advantage of this design approach is the independence of the optimization algorithm and the flow solver, making it possible to couple almost any flow solver with any type of optimization algorithm. Most flow solvers that are used for hypersonic flow analysis are based on the parabolized Navier-Stokes (PNS) equations and employ efficient
#### **1.4 Outline of Thesis**

space-marching techniques. Space-marching PNS flow solvers can model steady hypersonic flow as accurately as Navier-Stokes solvers and generally with less computation time, thus making them well suited to optimization of hypersonic flows.

A good optimization algorithm uses the minimum number of objective function evaluations to find the global minimum of the function. Many algorithms have been developed, ranging from simple gradient-search algorithms to stochastic-genetic algorithms. However, at present, no one algorithm has been identified as being the best for all aerodynamic design optimization problems. The choice of an appropriate optimization algorithm is largely problem dependent and involves consideration of issues such as robustness, rate of convergence, and global-search capabilities. No attempt is made in this thesis to perform a rigorous assessment of optimization algorithms to determine the most efficient optimization algorithm for the hypersonic design problems discussed earlier. Rather, the benefits and disadvantages of some commonly used optimization algorithms are discussed and a literature review of several optimization studies is presented. Based on this discussion, a relatively simple gradient-search optimization algorithm is selected to perform the optimization for the cases studied in this thesis.

# **1.4 Outline of Thesis**

The primary objective of this thesis was to develop a new computational design tool based on an efficient PNS flow solver and a gradient-based optimization algorithm, and apply it to the design of scramjets and hypersonic nozzles. The idea of coupling a PNS solver to an optimization algorithm and applying it to these aerodynamic design problems is not new, however, this thesis contains several original ideas and unique applications that the author has not seen in the published literature to date:

- Coupling a three-dimensional PNS flow solver with a Nelder-Mead optimization algorithm
- Optimizing the aerodynamic surfaces of a complete scramjet engine using a flow solver that models viscous and high temperature thermochemical gas effects
- Optimizing an axisymmetric nozzle contour for use in a reflected shock tunnel
- Optimizing a square cross-section nozzle contour

The development of the design tool and the applications listed above are presented in the remainder of this thesis. To guide the reader, a breakdown of the purpose and contents of following chapters is provided below.

**Chapter 2.** A discussion of the three-dimensional PNS flow solver that was developed for this study is given in this chapter. The solver employs a variety of computational techniques and models to accurately and efficiently simulate the flow mechanisms associated with scramjet engines and high enthalpy shock tunnel nozzles. A large amount of the time

associated with this thesis was spent developing this code and carrying out the numerous test cases that are presented in Appendix E.

**Chapter 3.** A review of the various optimization algorithms that have been coupled with flow solvers and used in the literature for aerodynamic design is presented in the third chapter. The benefits and deficiencies of several optimization algorithms and techniques are discussed, and the algorithm used to form the design tool in the current study is detailed. The chapter concludes with a review of several optimization studies that specifically address the design of scramjet engines and hypersonic nozzles.

**Chapter 4.** The first application of the optimization design tool is presented in the fourth chapter where the geometric design of a Mach 12 axisymmetric scramjet flow path is discussed. The scramjet design concept employed is the same wrap-around concept introduced at the beginning of Chapter 1. The focus of the optimization study was to increase the axial thrust of the design and to determine the predominant flow features that contribute to or degrade the performance of the engine.

**Chapter 5.** The second application of the design tool was the optimization of an axisymmetric Mach 7 nozzle for a small pulse flow wind tunnel. The design process used to generate the optimized nozzle contour is described in the fifth chapter. The chapter also investigates the effect of initial designs on the convergence to an optimal design, and the effect of varying simplex movement parameters in the optimization algorithm.

**Chapter 6.** The axisymmetric Mach 7 nozzle designed in the previous chapter was manufactured and tested for core flow Pitot pressure uniformity in the Small Shock Tunnel at The University of Queensland (known as the SST facility). The details of nozzle construction, how the testing was carried out, and the results of the testing are discussed in the sixth chapter. Pitot pressure surveys indicated that the test flow produced by the nozzle was of a high quality and that the design tool was substantially better than classical methods for designing nozzles.

**Chapter 7.** In this chapter, the ability of the design tool to optimize three-dimensional aerodynamic bodies is demonstrated. The application is to optimize the expansion contour of a square cross-section nozzle for the same small shock tunnel. A square cross-section nozzle was considered because flow disturbances from wall anomalies that might arise due to errors in manufacture are less focused in a square cross-section nozzle compared to an axisymmetric nozzle. The chapter starts with a review of the methods that have been used previously to design square cross-section nozzles. Then, three nozzles of different lengths are designed and subsequently optimized for maximum test core flow uniformity. All of the optimized designs showed a substantial improvement in the test core flow quality, however, the flow quality of the optimized short nozzle fell short of being acceptable for use in a pulse flow wind tunnel because of high cross-flow pressure gradients.

### **1.4 Outline of Thesis**

**Chapter 8.** The final chapter of the thesis presents an assessment of the computationallybased optimization design tool and recommendations for extending its capabilities. Conclusions that were made through the application of the design tool to each of the three design studies are presented separately at the end of the respective chapters rather than in this final chapter.

# **Computational Flow Solver**

This chapter is concerned with the development of a computationally efficient flow solver capable of accurately modelling steady three-dimensional flows through scramjet engines and hypersonic nozzles. The approach that was taken in developing the solver involved a simple and fast formulation that did not sacrifice accuracy. This approach makes coding simpler and increases solver speed to levels where it can be practically used for optimization problems requiring many trial solutions. The name given to the solver is *sm3d*.

The chapter starts with a description of the parabolized Navier-Stokes (PNS) equations, which are the governing equations used in sm3d. Also described is the spacemarching solution technique, which is a widely used method for solving the PNS equations. Following on from this introductory discussion is a review of the development of PNS solver schemes and an overview of the scheme and the other phenomenological models used in sm3d. The PNS equations and associated equations are then discussed in detail together with the discretization and integration methods that make up sm3d. The final section of this chapter discusses the grid generation techniques used in the solver. A collection of eight test cases is also presented in Appendix E, which serve to validate and verify the phenomenological models implemented within the solver.

# 2.1 Governing Equations & Space-Marching

The governing set of equations used in *sm3d* are the conservative parabolized Navier-Stokes equations (PNS). They are a reduced set of the full compressible Navier-Stokes equations (NS) that can be used to model viscous continuum flow where the inviscid region of the flow is supersonic. The compressible NS equations are a mixed set of elliptic-parabolic equations for steady flows that, in general, need to be treated with a time-marching technique to produce an accurate solution. The elliptic nature of the full equation set means information can propagate upstream in the flow. The PNS equations, on the other hand, are a mixed set of hyperbolic-parabolic equations (under certain conditions) and, assuming that there is no downstream influence, can be solved using an efficient space-marching technique. The efficiency of the PNS equation solver is largely a result of this technique.

Rudman & Rubin [188] conducted one of the earliest studies involving the use of the PNS equations. The PNS equations that these investigators derived and solved were applicable to both inviscid and viscous steady supersonic and hypersonic flow regions. The PNS equations were obtained by deleting all the viscous terms containing partial derivatives with respect to the streamwise direction from the steady NS equations. The resulting set of equations were significantly reduced in size and could be used to solve viscous-inviscid interaction problems with a fraction of the computation time used for solving the same problems with the NS equations. Korte [121] demonstrated that the results from a space-marching flow solver based on the PNS equations and the results from a time-marching NS solver show good agreement for steady supersonic and hypersonic viscous flow problems that do not have a strong downstream influence.

In order to maintain a stable solution scheme when solving the PNS equations, there are certain requirements that have to be maintained to conserve the streamwise hyperbolicparabolic nature of the equation set. The PNS equations can only be applied to flows where the inviscid region is supersonic and the streamwise velocity component is always positive. If the streamwise velocity is assumed to be aligned with one of the coordinate axes, then applications are limited to cases where the predominant flow direction is in the axial direction. This restriction can be avoided to some degree by using a generalised coordinate system [216, 121], however, it adds to the complexity of the code. An additional requirement is that the streamwise pressure gradient in the streamwise momentum equation be treated with a "stability technique" (see Section 2.5). The pressure term in the subsonic portion of boundary layers. Consequently, the term can cause the equation system to become unstable and produce spurious solutions commonly known as "departure solutions".

The space-marching technique, which is commonly used to solve the PNS equations, is a solution technique for steady flows where the region of influence is always downstream. The technique involves discretizing a computational domain into slices that are normal to the stream-wise direction and integrating the governing flow equations on each slice until a steady state is reached. A steady state solution is determined for the first upstream slice before marching to the next downstream slice. The outflow plane of the upstream slice is then used as the inflow plane to the next downstream slice. The procedure continues until the end of the domain is reached. Srinivas [201] showed that the computational time required for a steady state solution of a two-dimensional supersonic flow problem using a whole domain time-marching technique, can be reduced by an order of magnitude by using a space-marching solution technique. A similar gain is expected for three-dimensional flows. Computer memory requirements are also reduced for space-marching schemes since only enough slices to reconstruct the downstream face are required in memory. Therefore, the technique is memory efficient in comparison to a purely time-marching scheme that requires the storage of the whole computational domain.

# 2.2 Review of PNS Solvers

Various numerical solution techniques have been proposed to solve the PNS equations over the last 30 years. The most common approach has been to use finite-differences [217, 86]. In this approach, the spatial and temporal partial derivatives in the flow equations are replaced with discrete Taylor series expansions, resulting in an algebraic representation of the partial differential equations. Essentially, the partial derivatives are approximated by ratios of finite-differences between flow variables at discrete points within the flow domain. The higher order terms of the Taylor series expansions are ignored for computational efficiency, however, accuracy and stability are sacrificed as more terms are truncated.

Some of the first pioneering finite-difference implementations of the PNS equations were by Rudman & Rubin [188], Boynton & Thomson [30], and Cresci *et al.* [47]. All of these studies used an explicit representation of the finite-differences because of the simplicity in coding such a scheme. An explicit schemes contains only one unknown in the difference equation so that it may be evaluated in terms of known quantities. The alternative is to use an implicit scheme, where the difference equations are expressed with multiple unknowns requiring simultaneous solution. Implicit schemes are generally more efficient than explicit schemes for the PNS equations but are more difficult to code [217].

The trend following the early work on PNS solvers was to use iterative, implicit finitedifference schemes [186, 139]. These were then followed by more efficient non-iterative implicit schemes. Two schemes of note that employed non-iterative implicit schemes were those of Vigneron *et al.* [228] and Schiff & Steger [194]. These schemes were nearly identical except that Schiff & Steger used a "sublayer approximation" technique to calculate the subsonic pressure gradient and Vigneron *et al.* retained a stable fraction of the streamwise pressure gradient calculated when evaluating the streamwise momentum equations for subsonic flow (see Section 2.5). The two schemes also used different linearization procedures. Many schemes followed along the same lines as the two aforementioned schemes, with the majority being based on central-differencing in the crossflow plane. A shortcoming of central-differencing schemes was that oscillations in the flow solution often resulted from flow discontinuities such as shocks. To alleviate this, many schemes employed artificial dissipation to smooth out the oscillations. A disadvantage of these artificial dissipation schemes was that high quality solutions required user manipulation on a case by case basis. An alternative to using central-differencing for evaluating the partial derivatives is to use an upwinding scheme [157]. Upwind schemes have the ability to "capture shocks" without significant oscillations and require little or no artificial dissipation. A simple upwinding finite-difference formulation expresses differences as either forward or backward differences depending on the local wave speed. If the wave speed is positive (where the positive direction is left to right) then a backward-difference is used; similarly, if the wave speed is negative a forward-difference is used. Therefore, flow information can only propagate in the direction of the acoustic waves, hence, the term upwinding. Centraldifferencing schemes, in contrast, can propagate information from outside the domain of dependence.

Another class of upwind schemes use the solution of the unsteady shock tube problem (or Riemann problem) between data points rather than using differences to calculate the partial differentials. This approach was first proposed by Godunov who solved the Riemann problem exactly between data points [70]. Solving the Riemann problem exactly ensures that the physically correct propagation of information throughout the flow is accounted for in the numerical solution. However, solving the exact Riemann problem requires an iterative method and many computational calculations. Lawrence *et al.* [132, 131] created a faster scheme based on Godunov's scheme [70] by employing the non-iterative approximate Riemann solver of Roe [181] in an implicit finite-volume scheme. A modification of Roe's approximate Riemann solver was also used in the explicit finite-difference code of Korte & McRae [126].

Other well known approximate Riemann solvers are the flux-vector splitting schemes of Steger & Warming [210], Van Leer [227] and Liou & Steffen [137], and the fluxdifference splitting scheme by Osher [166] (see Tannehill *et al.* [218] for an explanation of flux-vector and flux-difference splitting). Despite the many upwind schemes available, Roe's scheme [181] seems to have gained the widest acceptance for the solution of the inviscid flux terms in the PNS equations due to its coding simplicity and accuracy. However, Roe's scheme does not strictly enforce the entropy condition, therefore, nonphysical expansion shocks can be admitted as part of the numerical solution. This circumstance can arise in sonic points of expansions, resulting in an artificial acceleration on the fluid [166, 229]. Osher's upwind scheme [166] is similar to Roe's [181], however, it has been shown to strictly satisfy the entropy condition [167] and, as a result, is thought to be more robust and accurate in comparison to Roe's scheme [69, 1]. The price paid for this increase in performance is the extra computational calculations required, which is why Osher's scheme is not as prevalent as Roe's scheme in the literature.

An efficient approach to making computationally intensive upwind schemes more practical was suggested by Toro [224]. Toro's linearized approximate Riemann solver [223] was coupled with an exact iterative solver, where the linearized solver was used

to solve regions of slowly varying data, and the exact solver was used for the remaining flow domain. The linearized solver involves few, and simple, arithmetic operations and is used for the majority of the flow domain, thereby, reducing the computational effort. By adopting this approach, the benefits of the robust solver are retained while reducing the computational effort. A similar approach is taken in *sm3d* where an Osher type upwind solver [107] is coupled with the linearized solver of Toro [223] for calculating the cross-stream inviscid fluxes (see Section 2.11.4). The resulting scheme is robust and efficient compared to other flux-difference schemes.

## 2.3 Overview of the Present Flow Solver

Finite-volume discretization is used in *sm3d* to solve the integral form of the PNS equations. The finite-volume approach is taken because it is inherently conservative and well suited to flows with discontinuities such as shocks. A finite-volume scheme discretizes the flow domain into discrete control volumes (or cells) and solves for the fluxes across the interfaces between adjacent cells. The conservative flow equations are then applied to update the average flow quantities within the cell. The metrics are evaluated at cell interfaces rather than at grid points as is the case for finite-differencing. The integral formulation of the PNS equations permits theoretically infinite gradients of flow properties at discontinuities. A time-dependent form of the integral equations is also used to explicitly march cross-flow slices forward in time to a steady state before marching in space to the next downstream slice. This approach has been taken in a number of other solvers [196, 201], but it contrasts with solvers based on the steady-flow formulation where the time derivatives do not appear [126, 122]. Even though the time-dependent approach requires an iteration in time to reach steady flow at each slice along the duct, it has the advantage that relatively large streamwise steps may be taken. This can be advantageous in difficult duct geometries where robust (and consequently computationally intensive) grid generation schemes must be used.

Another aspect of the formulation of sm3d that contrasts with most other spacemarching solvers is that the dimensional Cartesian form of the governing equations is retained in the code and the stored data. This approach has been used previously for blunt-body studies [179]. It leads to a simpler formulation in comparison to formulations that transform the governing equations to computational space. However, a penalty of this approach is that the code must handle the generalised cell geometry and the vector arithmetic.

The *sm3d* solver is made spatially third-order accurate in the cross-stream plane by using the "monotone upstream-centred scheme for conservation laws" (MUSCL) [226] to extrapolate the primitive flow variables at the cell interfaces. Anderson *et al.* [16] per-

formed a series of numerical experiments and found that extrapolation of the primitive variables and subsequent reconstruction of the fluxes provides better flow solutions compared to extrapolating the fluxes. The Osher type flux solver of Jacobs [107] is coupled to the efficient linearized flux solver of Toro [223] to calculate the cross-stream inviscid interface fluxes. Second-order fully upwind MUSCL extrapolation is also used in the streamwise direction to directly reconstruct the fluxes on the downstream faces of cells from the current and previous upwind slices. Numerical oscillations in the MUSCL scheme are suppressed with a minimum modulus limiter [87].

The thermochemical modelling capabilities of *sm3d* are currently limited to thermally perfect multi-species gas mixtures that are thermodynamically frozen or in thermodynamic equilibrium (also known as vibrational equilibrium for flows not undergoing ionization), undergoing non-equilibrium chemical reactions. A thermodynamic nonequilibrium model was not implemented into the solver largely because of the time constraints imposed on this study. Thermodynamic relations for gas species in thermal equilibrium are modelled with curve fits obtained from Oldenborg *et al.* [163]. There are also three other "fast" equilibrium models for gas mixtures implemented in the code. Reaction rates are determined from a temperature dependent Arrhenius law using rate data from various models [61, 29, 55, 183, 163].

An approximately-coupled integration technique (similar to that used by Wadawadigi *et al.* [232]) is used to solve for the chemical production terms and the flux vectors in the PNS equations. The chemical production rates are calculated for the cell averaged state followed by the calculation of the cell fluxes assuming frozen flow. The PNS equations are then integrated in time to obtain the new cell sate. The advantage of this approach is that the solution procedure for the PNS equations is unaffected by the size of the chemistry model and the solution method used to solve for the kinetic rates. The species production terms are marched forward in time using the same explicit time step as the PNS equations. This may result in very small time steps when computing flows with disparate time scales. However, the speed of the present code on modern "super-computers" does not necessitate the extra complexity of implicit methods for the chemistry.

The solver was given the capability of modelling turbulent, compressible boundary layers by implementing a modified Baldwin & Lomax algebraic eddy-viscosity turbulence model [20]. The modifications made to the model also made it possible to calculate the growth of turbulent boundary layers over a three-dimensional corner in the presence of strong vortical flows.

Prior to discussing details of the equations, discretization and integration methods that comprise *sm3d*, a list of the assumptions made is presented below.

• The flow is assumed to be steady and free of stream-wise separation regions.

- The transport of species due to diffusion is assumed to be negligible. Therefore, the diffusion velocity of all species is set to zero.
- The flow is assumed to be thermodynamically frozen or in thermodynamic equilibrium such that the specific internal energy of individual gas species is always a function of the translational temperature only,  $e = f(T_{\text{trans}})$ .
- The flow is assumed to always have a positive momentum value in the *x* direction, which is the space-marching direction and predominant flow direction. This restriction could have been removed by implementing a generalised coordinate system [216, 121], however, this approach adds extra complexity to the code and is not currently required.

# 2.4 Parabolized Navier-Stokes Equations

The integral form of the three-dimensional PNS equations for a chemically reacting, multi-species flow without body forces or external heat addition may be written as

$$\frac{\partial}{\partial t} \int_{V} \mathbf{U} dV + \oint_{S} \left( \mathbf{F_{i}} - \mathbf{F_{v}} \right) \cdot \hat{\mathbf{n}} dS = \int_{V} \mathbf{Q} dV \quad , \tag{2.1}$$

in the control volume V bounded by the surface S. The algebraic vector of dependent flow variables is

$$\mathbf{U} = \begin{bmatrix} f_i \rho \\ \rho u_x \\ \rho u_y \\ \rho u_z \\ \rho E \end{bmatrix} , \qquad (2.2)$$

the inviscid flux vectors is

$$\mathbf{F}_{\mathbf{i}} = \begin{bmatrix} f_{i}\rho u_{x} \\ \rho u_{x}^{2} + p \\ \rho u_{y} u_{x} \\ \rho u_{z} u_{x} \\ \rho E u_{x} + p u_{x} \end{bmatrix} \hat{i} + \begin{bmatrix} f_{i}\rho u_{y} \\ \rho u_{x} u_{y} \\ \rho u_{y}^{2} + p \\ \rho u_{z} u_{y} \\ \rho E u_{y} + p u_{y} \end{bmatrix} \hat{j} + \begin{bmatrix} f_{i}\rho u_{z} \\ \rho u_{x} u_{z} \\ \rho u_{y} u_{z} \\ \rho u_{z}^{2} + p \\ \rho E u_{z} + p u_{z} \end{bmatrix} \hat{k} , \quad (2.3)$$

and the viscous flux vector is

$$\mathbf{F}_{\mathbf{v}} = \begin{bmatrix} 0\\0\\0\\0\\0 \end{bmatrix} \hat{i} + \begin{bmatrix} 0\\\tau_{xy}\\\tau_{yy}\\\tau_{zy}\\u_{x}\tau_{xy} + u_{y}\tau_{yy} + u_{z}\tau_{zy} - q_{y} \end{bmatrix} \hat{j} + \begin{bmatrix} 0\\\tau_{xz}\\\tau_{yz}\\\tau_{zz}\\u_{x}\tau_{xz} + u_{y}\tau_{yz} + u_{z}\tau_{zz} - q_{z} \end{bmatrix} \hat{k}.$$
 (2.4)

The source term is

$$\mathbf{Q} = \begin{vmatrix} \dot{\omega}_{i} \\ 0 \\ 0 \\ 0 \\ 0 \end{vmatrix} , \qquad (2.5)$$

where  $(i = 1, 2, ..., N_S)$ . These equations specify the conservation of mass, three components of momentum, and total energy. The fluxes are separated into inviscid,  $\mathbf{F_i}$ , and viscous,  $\mathbf{F_v}$ , components where the streamwise direction is aligned with the *x*-axis or  $\hat{i}$ . These equations can be slightly modified to form the PNS equations for axisymmetric flow which are shown in Appendix A.

For a non-reacting gas, the total specific internal energy is defined by

$$E = e + \frac{1}{2}(u_x^2 + u_y^2 + u_z^2) \quad . \tag{2.6}$$

However, for reacting gas mixtures, the total energy includes the total formation enthalpy of the gases (see Eq. (2.27)). The formation enthalpy provides a mechanism for heat addition or absorption in chemical reactions and will be considered later (Section 2.6).

The viscous stresses are given by

$$\tau_{xx} = 0$$
  

$$\tau_{yy} = \frac{2}{3} \mu \left( 2 \frac{\partial u_y}{\partial y} - \frac{\partial u_z}{\partial z} \right)$$
  

$$\tau_{zz} = \frac{2}{3} \mu \left( 2 \frac{\partial u_z}{\partial z} - \frac{\partial u_y}{\partial y} \right)$$
  

$$\tau_{xy} = \mu \frac{\partial u_x}{\partial y} = \tau_{yx}$$
  

$$\tau_{xz} = \mu \frac{\partial u_x}{\partial z} = \tau_{zx}$$
  

$$\tau_{yz} = \mu \left( \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right) = \tau_{zy} , \qquad (2.7)$$

where  $\mu$  is the first coefficient of viscosity. This formulation of viscous stresses assumes negligible bulk viscosity since we are not concerned with the study of the structure of shock waves and absorption and attenuation of acoustic waves [219]. The viscous heat fluxes are

$$q_x = 0 ,$$
  

$$q_y = k \frac{\partial T}{\partial y} ,$$
  

$$q_z = k \frac{\partial T}{\partial z} .$$
(2.8)

The evaluation of the viscous transport coefficients,  $\mu$  and k, depend on the specific gas model and are modified when using an algebraic turbulence model. The evaluation of these terms will be covered in Section 2.8 & 2.9.

The  $\dot{\omega}_i$  terms in the source vector **Q**, are the production rates of species *i* in volume *V* due to the chemical reactions taking place in the volume. The equations used to evaluate these terms are given in Section 2.7.

# 2.5 Streamwise Pressure Gradient

When implementing a space-marching method for the PNS equations, it is necessary to either remove or modify the streamwise pressure gradient term in the streamwise flux vector (vector  $\hat{i}$  in Eq. (2.3)). An exact representation of the streamwise pressure gradient permits information to be propagated upstream through subsonic portions of the flow-field such as boundary layers. If this is the case, the subsonic areas of the flow become elliptic in nature and may cause exponentially growing solutions known as "departure solutions".

A simple method for preventing departure solutions is to omit the pressure gradient term completely from the PNS equations in the subsonic regions of the flow. This approach will result in a stable space-marching scheme only if there are minimal streamwise pressure gradients. Lubard & Helliwell [139] suggested retaining the pressure gradient term and using a backward-difference formula for the streamwise pressure gradient term in both the momentum and energy equations. This scheme prevents upstream information propagation if the minimum streamwise step size is not less than a limit which can be of the order of the thickness of the subsonic boundary layer [187]. Therefore, stable and accurate solutions are difficult to produce with such a method.

Rubin & Lin [186] proposed the "sublayer approximation" technique where the pressure gradient term in the subsonic viscous region is calculated at a supersonic point outside of the sublayer region. Schiff & Steger [194] applied this technique in a PNS code and found that is was also prone to departure solutions for various cases.

One of the most effective methods to stabilise the PNS equations in subsonic flow was by proposed by Vigneron *et al.* [228]. The stability analysis of the PNS equations performed by Vigneron *et al.* and later extended by Davis *et al.* [51] showed that only a

fraction  $(1 - \varepsilon)$  of the streamwise pressure term in the streamwise momentum equation, is responsible for the upstream propagation of information. If this fraction is dropped, the eigenvalues of the PNS equations will remain real, even in the subsonic regions thus maintaining the parabolic/hyperbolic nature of the governing equations and stabilising the space-marching procedure.

The remaining fraction,  $\varepsilon$ , is known as "Vigneron's coefficient" and is given as,

$$\varepsilon = 1, \qquad M_x \ge M_{\text{limit}} ,$$
  

$$\varepsilon = \frac{\Phi \gamma M_x^2}{1 + (\gamma - 1)M_x^2}, \quad M_x < M_{\text{limit}} ,$$
(2.9)

where the streamwise Mach number is denoted by  $M_x$  and the limiting Mach number is

$$M_{\rm limit} = \sqrt{\frac{1.0}{1.0 + \gamma(\Phi - 1.0)}} \quad . \tag{2.10}$$

The term  $\Phi$  is a safety factor which ranges from 0.75 for complex shock-boundary layer interactions to 1.0 for simple boundary layer flows where there is less uncertainty in determining the viscous stability limit (see Fig. 2.1).



Figure 2.1: Fraction of the streamwise pressure gradient versus Mach number [121].

The inviscid streamwise flux vector then becomes

$$\begin{bmatrix} f_i \rho u_x \\ \rho u_x^2 + \varepsilon p \\ \rho u_y u_x \\ \rho u_z u_x \\ \rho E u_x + p u_x \end{bmatrix} \hat{i}$$
(2.11)

Even though this approach only retains as much of the streamwise pressure gradient as a stability analysis permits, it is sometimes necessary to set the pressure gradient to 0 for the first few space-marching slices in a space-marching scheme (that is, set  $\varepsilon$  to 0) [195, 216]. The presence of a pressure gradient during the first few space-marching slices can cause solutions to become unstable. The number of slices that require the pressure gradient to be set to 0 depends on the step size and problem. A trial and error method is typically used to obtain the correct number of slices, however, 7 steps usually works well.

Other techniques for treating the streamwise pressure gradient have been proposed by various investigators [136, 33, 26, 187], however, Vigneron's seems to be the favoured approach for single sweep space-marching schemes amongst the computational community.

# 2.6 Thermodynamic Models

The PNS equations are supplemented with an equation of state which relates the pressure to the density and internal energy as

$$P = P(\rho, e) \quad . \tag{2.12}$$

The evaluation of this function depends on the thermodynamic model used to define the behaviour of the gas. The thermodynamic models used in *sm3d* all assume that the gas behaves as a perfect gas where intermolecular forces are considered negligible. The assumption of a perfect gas only becomes invalid at very high pressures ( $p \approx 1000$  atm) or at low temperatures ( $T \approx 30$  K). Under these conditions the distances between molecules becomes small and intermolecular forces of attraction and repulsion become significant. In the vast majority of gas-dynamic applications, the temperatures and pressures are such that the perfect gas assumption can be applied with confidence [7].

For a mixture of perfect gases

$$p = \rho \tilde{R}T \quad . \tag{2.13}$$

where  $\tilde{R}$  is the mixture gas constant which is defined as

$$\tilde{R} = \sum_{i=1}^{N_S} \frac{\rho_i}{\rho} R_i = \sum_{i=1}^{N_S} f_i R_i \quad .$$
(2.14)

Dalton's law of partial pressures also applies to perfect gases where the pressure of a gas mixture is equal to the sum of the partial pressures. This law can be expressed as

$$p = \sum_{i=1}^{N_S} \rho_i R_i T = \rho \tilde{R} T \quad , \tag{2.15}$$

where the density of the mixture is

$$\rho = \sum_{i=1}^{N_S} \rho_i \quad .$$
 (2.16)

These equations are applicable for both reacting and nonreacting perfect gas mixtures which are both addressed in the following sections. We now consider the various thermodynamic models of perfect gases used to define Eq. (2.12).

### 2.6.1 Calorically perfect gas model

The simplest thermodynamic model available in sm3d is for a calorically perfect gas. A calorically perfect gas is one where only translational and rotational modes of energy contribute to the total internal energy of the gas. For such a gas, the enthalpy and internal energy both hold linear relationship with the temperature of the gas such that,

$$h = C_p T$$
 and  $e = C_v T$ . (2.17)

The specific heats  $C_p$  and  $C_v$  are constant for a calorically perfect gas and as a result, the ratio of specific heats  $\gamma = C_p/C_v$ , is also constant. The equation of state can then be simply expressed as,

$$p = \rho(\gamma - 1)e \quad . \tag{2.18}$$

The calorically perfect model is usually adequate for low enthalpy flows where temperatures remain relatively low (below 1000 K for air [12, 79]). At higher temperatures the specific heats are no longer constant and become functions of temperature due to the excitation of the vibrational and electronic energy modes.

### 2.6.2 Vibrational Equilibrium Model

High temperature gas flow is often associated with the excitation of vibrational and electronic energy modes in individual species as well as the dissociation and recombination of chemical bonds within molecules. Electronic excitation occurs in most molecules and atoms at temperatures exceeding 6000 K [80]. For this reason electronic excitation is not considered in the present study since the temperatures in the scramjet engines and pulse facility nozzles being considered are well below this limit. However, vibrational excitation and chemical dissociation/recombination can be quite prevalent between 1000K and 6000K. This section deals with the modelling of equilibrium vibrational excitation within gas mixtures leaving the modelling of chemical dissociation/recombination to the following section (see Section 2.7).

#### 2.6 Thermodynamic Models

The sensible energy (energy based on statistical mechanics [8]) of single species and non-reacting gas mixtures in vibrational equilibrium, can be derived as a function of static temperature. Solutions of these functions for various species can be found in tables where the molar thermodynamic properties are listed against temperature [41, 147]. For computational applications it is common to fit a polynomial equation to the tabulated specific heat data and integrate this equation to get the molar thermodynamic quantities  $H^o$  and  $S^o$ . The nominal polynomial curve fits used for *sm3d* are those found in Oldenborg *et al.* [163] and the polynomial coefficients for these curves are reproduced in Appendix B. The thermodynamic curve fits and reaction data for all the predominant species involved in hydrogen combustion in air up to a temperature of 6000 K are presented in this source.

The polynomial used for the molar  $C_p^o$  is expressed as,

$$C_p^o/R^o = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 , \qquad (2.19)$$

where a different set of polynomial coefficients,  $a_1...a_7$ , are used for each species. Integration of the expression for  $C_p^o$  will give the value of molar enthalpy at temperature T as

$$H^{o} = \int_{T_{R}}^{T} C_{p}^{o} dT + D \quad , \qquad (2.20)$$

where D is the integration constant that sets enthalpy to zero at the reference temperature  $T_R$ . Substituting Eq. (2.19) into Eq. (2.20) and solving gives,

$$H^{o}/R^{o} = -a_{1}T^{-1} + a_{2}\ln T + a_{3}T + a_{4}T^{2}/2 + a_{5}T^{3}/3 + a_{6}T^{4}/4 + a_{7}T^{5}/5 + a_{9} \quad .$$
(2.21)

The curve fits listed in reference [163] are referenced to a temperature of 298.15 K such that the integration constant  $a_9R^o$  in Eq. (2.21) is equivalent to D plus the heat of formation at the standard reference temperature of 298.15 K. This poses a problem computationally since we require the sensible energy of the gas to always maintain a positive value for all temperatures. To maintain this condition, the expression for enthalpy was referenced to 0 K by deducting the heat of formation at 298.15 K and adding the difference in enthalpy between 0 K and 298.15 K. In this form, all the species sensible enthalpies and thus sensible internal energies, will be 0 at a temperature of 0 K. The formation enthalpy at 0 K is not added here since it is accounted for later in the total energy equation (2.27).

If the molar specific heat at constant pressure in Eq. (2.19) is divided by T and then integrated from temperature  $T_R$  to T, the difference in entropy between these two temperatures is given as

$$S^{o} = \int_{T_{R}}^{T} \frac{C_{p}^{o}}{T} dT + D \quad .$$
 (2.22)

The corresponding polynomial function is,

$$S^{o}/R^{o} = -a_{1}T^{-2}/2 - a_{2}T^{-1} + a_{3}\ln T + a_{4}T + a_{5}T^{2}/2 + a_{6}T^{3}/3 + a_{7}T^{4}/4 + a_{10}$$
(2.23)

where this function evaluates to the entropy difference from a reference state of 0 K using the polynomial coefficients from reference [163].

The Gibbs free energy,

$$G^o = H^o - TS^o \quad , \tag{2.24}$$

is used to calculate the equilibrium constant for a particular reaction as shown later in Eq. (2.38).

The molar internal energy for each species can also be calculated using the equation

$$E^o = H^o - R^o T \quad . \tag{2.25}$$

For a gas mixture, the specific sensible internal energy in J/kg can be computed from the individual species molar values at a given temperature from the equation

$$e = \sum_{i=1}^{N_S} f_i \frac{E_i^o}{M_i} \quad , \tag{2.26}$$

where  $f_i$  is the mass fraction of species *i* and is equivalent to  $\rho_i/\rho$ .

The total specific energy is given as

$$E = e + \frac{1}{2}(u_x^2 + u_y^2 + u_z^2) + \sum_{i=1}^{N_S} \frac{(\Delta H_f^o)_{T_R,i}}{M_i} f_i \quad ,$$
(2.27)

where  $(\Delta H_f^o)_{T_R,i}$  is the molar heat of formation of species *i* at the reference temperature  $T_R = 0$  K. This term provides the mechanism for energy absorption and release due to chemical reactions.

The other common method for accounting for the heat of reaction is to use a published value of the heat of reaction for a particular reaction. The energy added or consumed by the reaction is then determined by multiplying the heat of reaction term by the reaction

#### 2.6 Thermodynamic Models

rate. These quantities are then summed over all reactions and added as an energy source term in the governing equations (Eq. (2.5)). The method of calculating the heat of reaction from heats of formation is used in *sm3d* because heat of reaction data is not as consistent between published data sets.

In Eq. (2.27), the total specific energy is written as a function of temperature, flow speed and species mass fractions. However, in the solution procedure, it is necessary to calculate the temperature, given the total specific energy, flow speed and mass fractions. Since the energy equation for vibrational equilibrium is expressed as a polynomial and can not be rearranged to give a simple expression for the temperature, an iterative secant method is used to find the temperature to within a set tolerance. To increase the convergence rate of the secant method, an initial guess is obtained from a look up table of energies and corresponding temperatures for the gas mixture contained within the cell. The look up table is only used for computational cells where no previous time step temperature exists for the cell.

Once the temperature of the gas mixture has been determined, the remaining nonconservative properties can be calculated. The pressure is given by Dalton's law as discussed earlier (see Eq. 2.15). The frozen speed of sound [76] is used for all computations in the current code and is defined as

$$a^{2} = \gamma \frac{p}{\rho} = \left(\frac{C_{p}}{C_{p} - \tilde{R}}\right) \tilde{R}T \quad , \qquad (2.28)$$

where

$$C_p = \sum_{i=1}^{N_S} f_i \frac{C_{p,i}^o}{M_i} \quad .$$
(2.29)

Note that the  $\gamma$  used is the ratio of specific heats corresponding to the internal energy being in thermodynamic equilibrium.

### 2.6.3 Fast Equilibrium Models

In addition to the general vibrational equilibrium model presented above, three extra models have been included in the code to model nitrogen and air in thermodynamic equilibrium. These models have been specifically written to be computationally efficient. An iterative solver is included in each model to solve for temperature given the specific internal energy and density.

The first model is for non-dissociating nitrogen in vibrational equilibrium and is limited to gas temperatures where nitrogen dissociation does not occur (approximately below 4000K at 1 atm.). The specific internal energy of nitrogen is given by a simple relation that sums the components of translational and vibrational energy as

$$e_{N_2} = \left(2.5 + \frac{\frac{\theta_{\text{vib}}}{T}}{\exp\left(\frac{\theta_{\text{vib}}}{T}\right) - 1.0}\right) R_{N_2}T \quad , \tag{2.30}$$

where  $\theta_{\rm vib}$  is the characteristic temperature for the vibrational mode of nitrogen (3389 K).

The second model is used to calculate the mixture internal energy of dissociating nitrogen in thermodynamic equilibrium up to temperatures of 15000 K [171]. Given a temperature and density, it works out the equilibrium mass fractions of N and N<sub>2</sub>, and then the mixture internal energy using a series of curve fits for several temperature ranges. This model has limited applicability at large temperatures because it does not consider ionization.

Lastly, an equilibrium air model is included which models non-dissociating air in thermodynamic equilibrium [203]. The model is based on a set of curve fits for oxygen and nitrogen.

### 2.7 Chemistry Model

The species production terms  $\dot{\omega}_i$  in Eq. (2.1) represent the production rate of species *i* in a cell volume due to the chemical reactions taking place in that cell. All of the reaction schemes used in this thesis for modelling hydrogen combustion are presented in Appendix C. Each of these schemes is made up of reactions describing paths for dissociation and recombination of the chemical species present in the test flow. Each reaction set has the general form,

$$\sum_{i=1}^{N_S} \alpha'_{ij} Z_i \xrightarrow{\longrightarrow} \sum_{i=1}^{N_S} \alpha''_{ij} Z_i \qquad (j = 1, 2, ..., N_R) \quad , \tag{2.31}$$

where  $Z_i$  are the chemical symbols and  $\alpha', \alpha''$  are the reactant and product stoichiometric coefficients respectively. Total species production rates,  $\dot{\omega}_i$ , are determined by summing the contributions from each contributing reaction. Each reaction is assumed to be governed by a "law-of-mass-action" expression where the rate constants can be determined from a temperature dependent Arrhenius law. The net rate of change of concentration of species *i* by reaction *j* is given by

$$(\dot{C}_i)_j = (\alpha_{ij}'' - \alpha_{ij}') \left( k_{f,j} \prod_{l=1}^{N_S} C_l^{\alpha_{lj}'} - k_{r,j} \prod_{l=1}^{N_S} C_l^{\alpha_{lj}''} \right) \quad , \tag{2.32}$$

where  $k_f, k_r$  are the forward and reverse reaction rates respectively and C are the species concentrations. The rate change in concentration of species i by  $N_R$  reactions is then found by summing the contributions from each reaction which is written as

$$\dot{C}_i = \sum_{j=1}^{N_R} (\dot{C}_i)_j$$
 (2.33)

Finally, the production rate of species i in kg/(m<sup>3</sup>.s), is found from

$$\dot{\omega}_i = \dot{C}_i M_i \quad , \tag{2.34}$$

where M is the molecular weight in kg/mol.

The forward reactions rates are computed from the modified Arrhenius law

$$k_{f_j} = A_j T^{N_j} \exp\left(\frac{-\theta_j}{T}\right) \quad . \tag{2.35}$$

for each reaction j, where  $A_j$  and  $N_j$  are constants for reaction j, and  $\theta_j$  is the activation temperature in Kelvins. The activation temperature is equal to the activation energy of the reaction divided by  $R^o$ . The reverse rate can be found given the forward rate and equilibrium constant  $K_j$  for each reaction j as

$$k_{rj} = \frac{k_{fj}}{K_j} \quad . \tag{2.36}$$

The equilibrium constant is a function of the difference between Gibbs free energy of the reactants and products and temperature as given by

$$K_j = \left(\frac{R^o T \ 10^6}{p_{\rm atm}}\right)^{l_j} \exp\left(\frac{-\Delta G_j^o}{R^o T}\right) \quad . \tag{2.37}$$

In the above equation,  $l_j$  is equal to the integer sum of the stoichiometric coefficients of the reactants minus the sum of coefficients of the products for reaction j. The standard Gibbs free energy difference for the reaction j is,

$$\Delta G_j^o = \sum_{i=1}^{N_S} \alpha_{ij}'' G_i^o - \sum_{i=1}^{N_S} \alpha_{ij}' G_i^o \quad .$$
(2.38)

## 2.8 Transport Coefficients

The coefficients of viscosity and thermal conductivity contained in the viscous terms of Eq. (2.1) are composed of laminar and turbulent components.

$$\mu = \mu_{\text{lam}} + \mu_{\text{turb}} \tag{2.39}$$

$$\frac{k}{C_p} = \frac{\mu_{\text{lam}}}{Pr} + \frac{\mu_{\text{turb}}}{Pr_{\text{turb}}}$$
(2.40)

If the flow is completely laminar then the turbulent components are set to 0.

The laminar coefficient of viscosity is calculated using Sutherland's simple formula for single species gases [211]. The formula can be written as

$$\mu_{\rm lam} = A \frac{T^{3/2}}{T+B} \tag{2.41}$$

where A and B are gas dependent constants and T is the static temperature of the gas in Kelvins. The coefficients for various gases are listed in Table 2.1 with a temperature range

Gas	A	В	T range for
	$kg.m^{-1}.s^{-1}.K^{-0.5}$	Κ	2% error
Hydrogen, H <sub>2</sub>	$6.899 \times 10^{-7}$	97	220-1100
Helium <sup>*</sup> , He	$1.461 \times 10^{-6}$	79	
Carbon Monoxide, CO	$1.503 \times 10^{-6}$	136	130-1500
Nitrogen, N <sub>2</sub>	$1.400\times10^{-6}$	107	100-1500
Air	$1.461 \times 10^{-6}$	111	170-1900
Oxygen, O <sub>2</sub>	$1.753\times10^{-6}$	139	190-2000
Argon, Ar	$1.964 \times 10^{-6}$	144	120-1500
Carbon Dioxide, CO <sub>2</sub>	$1.503\times10^{-6}$	222	190-1700

Table 2.1: Sutherland's viscosity coefficients from [85], [40]\*.

of applicability. The Sutherland formula is valid for single component gases, however, air is included because its two principal components, oxygen and nitrogen, are nearly identical diatomic molecules. For gas mixtures that are composed of dissimilar components, the mixture viscosity varies strongly with species concentration.

The viscosity of a gas mixture is given by the approximate mixing rule of Wilke [238].

Pure species viscosities are combined using the equation

$$\mu_{\text{lam}} = \sum_{i=1}^{N_s} \frac{X_i \mu_i}{\sum_{j=1}^{N_s} X_j \phi_{ij}} \quad , \tag{2.42}$$

where  $X_i$  is the mole fraction of species *i*, and  $\phi_{ij}$  is defined as

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_i}{M_j} \right)^{-\frac{1}{2}} \left[ 1 + \sqrt{\frac{\mu_i}{\mu_j}} \left( \frac{M_j}{M_i} \right)^{\frac{1}{4}} \right]^2 \quad . \tag{2.43}$$

The mole fractions are computed from the species densities and molecular weights.

$$X_i = \frac{\rho_i/M_i}{\sum_{j=1}^{N_S} \rho_j/M_j}$$
(2.44)

The individual species coefficients of viscosity,  $\mu_i$ , in Eq. (2.42) are given by an equation derived by Hirschfelder *et al.* [88], rather than the Sutherland's equation. The Hirschfelder *et al.* equation was used because the constants in the equation are readily available for a wide range of species. However, the number of numerical computations required to solve this equation is higher than that of Sutherland. The equation proposed by Hirschfelder *et al.* [88] is

$$\mu_i = 2.6693 \times 10^{-6} \frac{\sqrt{M_i T}}{\sigma_i^2 \Omega_i^{(2,2)}} \quad , \tag{2.45}$$

where  $\sigma_i$  is the collision diameter in  $(\stackrel{\circ}{A})$ , and  $\Omega^{(2,2)}$  is the elastic collision integral of species *i*. The collision integral for species *i* can be expressed as an empirical function [160] of the reduced temperature  $T^*$ 

$$\Omega_i^{(2,2)} = [A(T^*)^{-B}] + C[\exp(-DT^*)] + E[\exp(-FT^*)] \quad , \tag{2.46}$$

where the reduced temperature is

$$T^* = \frac{k_B T}{\epsilon_i} \quad , \tag{2.47}$$

and the constants are

$$A = 1.16145, \quad B = 0.14874, \quad C = 0.52487,$$
  
 $D = 0.77320, \quad E = 2.16178, \quad \text{and} \quad F = 2.43787.$  (2.48)

Equation (2.46) is applicable over the range  $0.3 \le T^* \le 100$  with an average deviation of only 0.064 percent. For species that take part in hydrogen combustion with air, this reduced temperature range translates to a real temperature range of approximately 87 K  $\le T \le 3700$  K. This range is based on the heaviest and lightest substances in the range of species present.

The collision diameter  $\sigma_i$  and the characteristic energy  $\epsilon_i$  are molecular constants for the Lennard-Jones 6-12 intermolecular potential function. Tabulated potential parameter data ( $\epsilon_i/k_B$  and  $\sigma_i$ ) for various species are found in [212]. The potential parameters for the species that are involved in air-hydrogen combustion are listed in Appendix D.

The thermal conductivity coefficient  $k_{\text{lam}}$  is calculated for a single species gas using the Reynolds analogy assuming a constant Prandtl number.

$$k_{\rm lam} = \frac{\mu_{\rm lam} C_p}{Pr} \tag{2.49}$$

For multi-species gas mixtures, the same equation is used where a constant Prandtl number is assumed and  $\mu_{\text{lam}}$  and  $C_p$  are the mixture values.

# 2.9 Turbulent Viscosity and Thermal Conductivity

A popular approach for modelling turbulent hypersonic flow is to employ algebraic turbulence models rather than one-equation and two-equation models. Algebraic turbulence models are attractive because of their efficiency, simplicity, and robustness. Also, more sophisticated models require larger storage space and a greater number of numerical computations. Complicated turbulence models have been shown to offer only minimal flow modelling improvements for attached flows [95, 231, 49].

Two well known algebraic models were developed by Cebeci & Smith [37] (CS) and Baldwin & Lomax [20] (BL). An evaluation of these models for supersonic and hypersonic flows is presented by Shirazi & Truman [195]. This study shows that the differences in the two models are due to the near-wall damping term used, the outer eddy-viscosity formulation, and the effects of outer-layer intermittency. They are both two layer eddyviscosity model formulations, primarily differing in the choice of length and velocity scales in the outer layer. The CS turbulence model uses the displacement thickness as the length scale, and the BL turbulence model uses a length scale based on the vorticity distribution. For complex separated flows it is not a simple matter to determine the displacement thickness, so for this reason the BL model is used in *sm3d*. The BL model expresses the turbulent viscosity coefficient  $\mu_{turb}$  in Eq. 2.39, as a two layer formulation given by

$$\mu_{\text{turb}} = \begin{cases} (\mu_{\text{turb}})_{\text{inner}} & \text{if } d \le d_c \\ (\mu_{\text{turb}})_{\text{outer}} & \text{if } d > d_c \end{cases} ,$$
(2.50)

where d is the local distance measured normal to the body surface, and  $d_c$  is the smallest value of d at which the values from the inner and outer region formulae are equal (see Fig. 2.2).



Figure 2.2: Switching from inner to outer value of eddy viscosity.

The body surface distance for three-dimensional right angle corner flows can be approximated with a "modified distance" equation that was suggested by Hung & MacCormack [98]. The equation for the "modified distance" is

$$d = \frac{2yz}{(y+z) + \sqrt{y^2 + z^2}} \quad . \tag{2.51}$$

This equation accounts for the size of the turbulent eddy or the turbulent mixing length near a corner under the influence of both the y and z walls.

The inner layer turbulent viscosity in Eq. (2.50) is given by,

$$(\mu_{\rm turb})_{\rm inner} = \rho l^2 |\omega| \quad , \tag{2.52}$$

where

$$l = kd[1 - \exp(-d^{+}/A^{+})] \quad . \tag{2.53}$$

The square bracketed term in the above equation is the van Driest damping term (denoted as D from here on). This is the original damping term that appeared in the paper by Baldwin & Lomax [20], which was derived for incompressible flow. The damping term can be modified to include compressibility effects that can be quite prevalent in the inner layer

of hypersonic flows. The van Driest damping term for compressible flow as presented by Cebeci & Smith [37] is,

$$D = 1 - \exp\left[\frac{-d^+(\rho/\rho_{\text{wall}})^{1/2}(\mu_{\text{wall}}/\mu)}{A^+}\right] \quad . \tag{2.54}$$

The compressible damping term was used in *sm3d* since it gives appreciably better results for turbulent compressible flow [195]. Shirazi & Truman [195] note that the difference in results between the CS model and the BL model is almost entirely due to the form of damping used. For corner flows, calculation of the damping term is based on the proximity to neighbouring walls. Referring to Fig. 2.3, the damping term in regions 1 and 2 is evaluated from the wall y = 0, and in regions 3 and 4, the wall z = 0.



Figure 2.3: Division of computational space for turbulent calculations.

The law of the wall coordinate in the damping term,  $d^+$ , is given by

$$d^{+} = \frac{\sqrt{\rho_{\text{wall}}\tau_{\text{wall}}} \ d}{\mu_{\text{wall}}} \tag{2.55}$$

and the magnitude of vorticity in three-dimensions is equal to,

$$|\omega| = \sqrt{\left(\frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial v}{\partial z} - \frac{\partial w}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial z}\right)^2} \quad . \tag{2.56}$$

where the streamwise terms have been neglected. For the outer layer,

$$(\mu_{\rm turb})_{\rm outer} = K C_{\rm cp} \rho F_{\rm wake} F_{\rm Kleb}(d) \quad , \tag{2.57}$$

where  $F_{\text{wake}}$  is the smaller of

$$F_{\text{wake}} = \begin{cases} d_{\max} F_{\max} \\ C_{\text{wk}} d_{\max} u_{\text{diff}}^2 / F_{\max} \end{cases}$$
(2.58)

The term  $d_{\text{max}}$  is the value of d corresponding to the maximum value of F,  $F_{\text{max}}$ , where

$$F(d) = d|\omega|D \tag{2.59}$$

and  $F_{\text{Kleb}}$  is the Klebanoff intermittency factor given by

$$F_{\rm Kleb} = [1 + 5.5 (C_{\rm Kleb}/d_{\rm max})^6]^{-1} \quad . \tag{2.60}$$

The search for  $F_{\text{max}}$  and its corresponding  $d_{\text{max}}$  in corner regions proceeds outward from the wall as shown in Fig. 2.3. The search proceeds either from y = 0 for region 4, or from z = 0 for region 1. The values of  $F_{\text{max}}$  in regions 2 and 3 are constants, equal to the value of  $F_{\text{max}}$  at m and n, respectively.

The quantity  $u_{\text{diff}}$  in Eq. (2.58) is the difference between maximum and minimum total velocity along a line of ascending d. The value of  $u_{\text{diff}}$  for boundary layer flows where the minimum velocity is 0 is given by

$$u_{\text{diff}} = (\sqrt{u^2 + v^2 + w^2})_{\text{max}}$$
 (2.61)

Transition to turbulence can be simulated by setting the computed value of turbulent viscosity,  $\mu_{turb}$ , equal to zero until the maximum in the profile normal to the wall is less than a specified value, that is,

$$\mu_{\text{turb}} = 0.0 \quad \text{if} \quad (\mu_{\text{turb}})_{\text{max. in profile}} < C_{\text{mutm}} \ \mu_{\infty} \quad .$$
(2.62)

The values of the constants appearing in Eqs. (2.53) to (2.62) are listed in [20] as

$$A^{+} = 26, \qquad C_{wk} = 1.0, \qquad (2.63)$$

$$C_{cp} = 1.6, \qquad k = 0.4, \qquad (2.63)$$

$$C_{Kleb} = 0.3, \qquad K = 0.0168, \qquad Pr_{turb} = 0.9, \qquad C_{mutm} = 14 .$$

Two modifications proposed by Degani & Schiff [52] were made to the BL model to increase the accuracy of modelling cross-stream separated flow regions. The first modification involved a method for determining the length scale in strong vortical flows. Strong

vortical flows can exist in regions of large separated boundary layers. In these types of vortical flow, two or more maximum values of the function F(d) (see Eq. (2.59) ) can exist with the outermost maximum being the largest. The selection of the largest  $F_{\text{max}}$  can result in an outer eddy viscosity that is as much as two orders of magnitude too high. To avoid this, Degani & Schiff [52] selected the first maximum closest to the wall where the value of F(d) drops to less than 90% of the local maximum as d increases (see Fig. 2.4).



**Figure 2.4:** Selection of correct F(d) in separated flow.

The second modification proposed by Degani & Schiff [52] simplifies the determination of  $F_{\text{max}}$  and  $d_{\text{max}}$  at separation points. The  $F_{\text{max}}$  value can rapidly increase at separation points due to the merging of recirculating flow from vortex structures and attached boundary layers. This merging produces high values of  $F_{\text{max}}$  at the outer regions of the merging region and blends the inner peak in  $F_{\text{max}}$  such that it can not be determined. On each ray of d (except on symmetry planes), a cutoff distance is specified in terms of the  $d_{\text{max}}$  value from the previous ray

$$d_{\rm cutoff}(\zeta) = 1.5 \, d_{\rm max}(\zeta - \Delta \zeta) \quad , \tag{2.64}$$

where  $\zeta$  is the coordinate along the wall in the cross flow plane. The distance  $\Delta \zeta$  is the distance between cell centres. If no peak in F(d) is found along a ray for  $d \leq d_{\text{cutoff}}$ , the values of  $F_{\text{max}}$  and  $d_{\text{max}}$  are taken from those found on the previous ray.

Once the turbulent viscosity coefficient is determined, the coefficient of thermal conductivity is calculated using Eq. (2.39). The turbulent Prandtl number is assumed to be 0.9 for both reacting and non-reacting systems.

### 2.10 Finite-Volume Discretization

The integral in Eq. (2.1) is evaluated over the computational domain in finite-volumes. These volumes are hexahedral cells as shown in Fig. 2.5. If the cell volumes are denoted V and the area of each face as dS, then the integral Eq. (2.1) can be written as

$$V\frac{\partial < \mathbf{U} >}{\partial t} + \oint_{S} \mathbf{F} \cdot \hat{\mathbf{n}}_{\mathbf{x}} dS + \oint_{S} \mathbf{F} \cdot \hat{\mathbf{n}}_{\mathbf{y}} dS + \oint_{S} \mathbf{F} \cdot \hat{\mathbf{n}}_{\mathbf{z}} dS = \int_{V} \mathbf{Q} dV, \qquad (2.65)$$

where  $\langle \mathbf{U} \rangle$  are the cell averaged values of the conserved variables stored for each cell at the centroid. Applying this equation to a six-sided cell and using average fluxes at the mid-points of each interface, the semi-discrete approximation to the governing equations becomes,

$$\frac{d < \mathbf{U} >}{dt} + \frac{1}{V} \left[ \overline{\mathbf{F}}_{ix-\frac{1}{2}} \cdot \hat{\mathbf{n}}_{ix-\frac{1}{2}} \, dS_{ix-\frac{1}{2}} + \overline{\mathbf{F}}_{ix+\frac{1}{2}} \cdot \hat{\mathbf{n}}_{ix+\frac{1}{2}} \, dS_{ix+\frac{1}{2}} + \mathbf{F}_{iy-\frac{1}{2}} \cdot \hat{\mathbf{n}}_{iy-\frac{1}{2}} \, dS_{iy-\frac{1}{2}} + \overline{\mathbf{F}}_{iy+\frac{1}{2}} \cdot \hat{\mathbf{n}}_{iy+\frac{1}{2}} \, dS_{iy+\frac{1}{2}} + \mathbf{F}_{iz+\frac{1}{2}} \cdot \hat{\mathbf{n}}_{iz+\frac{1}{2}} \, dS_{iz+\frac{1}{2}} \right] = \langle \mathbf{Q} \rangle \quad .$$
(2.66)

To evaluate the terms is this equation, the cell geometry is defined by the cell face normals, areas, and volumes. The Cartesian coordinate system (x, y, z) is used to define the positions of the cell vertices along with the normalized  $(\xi, \eta, \zeta)$ -coordinate system (see Fig. 2.5). The marching direction  $\xi$  is approximately aligned with the supersonic flow direction. The dashed vertices (a', b', c', d') define the upstream face of the cell while the undashed vertices define the corresponding downstream face.

Cell faces that have all of their vertices in a single  $\xi = constant$  plane are called *XFaces* within the code. *YFaces* and *ZFaces* have all of their vertices in  $\eta = constant$  and  $\zeta = constant$  planes respectively. The cycle *abcd* is chosen to correspond to an *XFace* having its unit normal positive in the  $\xi$  (streamwise) direction (see Fig. 2.6).



Figure 2.5: Finite-volume cell with coordinate directions and vertex labels.



Figure 2.6: XFace, YFace and ZFace vertices with unit normal and tangent vectors.

To get the geometric properties of an XFace, four edge vectors are defined as

The face is split into two triangular facets and the area vectors

$$\overline{\mathbf{A}}_{1} = \overline{\mathbf{ad}} \times \overline{\mathbf{ab}}$$

$$\overline{\mathbf{A}}_{2} = \overline{\mathbf{cb}} \times \overline{\mathbf{cd}}$$

$$(2.68)$$

are computed, with the average area vector of the face being defined as

$$\overline{\mathbf{A}} = \frac{1}{2} \left( \overline{\mathbf{A}}_1 + \overline{\mathbf{A}}_2 \right) \quad . \tag{2.69}$$

From this, the nominal surface area of the face is

$$dS_{ix+\frac{1}{2}} = |\overline{\mathbf{A}}| \quad , \tag{2.70}$$

and the corresponding unit normal is

$$\hat{\mathbf{n}}_{ix+\frac{1}{2}} = \frac{\overline{\mathbf{A}}}{|\overline{\mathbf{A}}|} \quad . \tag{2.71}$$



Figure 2.7: Finite-volume cell showing the unit normal at each interface.

Two tangent vectors can then be defined as

$$\hat{\mathbf{t}}_1 = \frac{\hat{\mathbf{n}} \times \overline{\mathbf{ad}}}{|\hat{\mathbf{n}} \times \overline{\mathbf{ad}}|} , \quad \hat{\mathbf{t}}_2 = \hat{\mathbf{n}} \times \hat{\mathbf{t}}_1 .$$
 (2.72)

Similar quantities can be defined for the YFaces using vertices cc'b'b and the ZFaces using vertices abb'a' (see Fig. 2.6).

The volume of each cell is computed by summing the volume of the six tetrahedrons that are contained within the cell (see Fig. 2.8). The volume of each tetrahedron is computed using a vector triple product

$$V_{it} = \frac{1}{6} \,\overline{\mathbf{d}} \cdot \left(\overline{\mathbf{a}} \times \overline{\mathbf{b}}\right) \,\,, \tag{2.73}$$

and the centroid is evaluated as an average of the vertex coordinates

$$\overline{\mathbf{P}}_{it} = \frac{1}{4} \left( \overline{\mathbf{P}}_1 + \overline{\mathbf{P}}_2 + \overline{\mathbf{P}}_3 + \overline{\mathbf{P}}_4 \right) \quad , \tag{2.74}$$

where  $\overline{\mathbf{P}}_1$  to  $\overline{\mathbf{P}}_4$  are the position vectors of the vertices (see Fig. 2.9). The original (hexahedral) cell volume is then evaluated as

$$V = \sum_{it=1}^{6} V_{it} \quad , \tag{2.75}$$

and the centroid is defined as

$$\overline{\mathbf{P}} = \frac{1}{V} \sum_{it=1}^{6} \overline{\mathbf{P}}_{it} V_{it} \quad .$$
(2.76)

# 2.11 Flow-Field Reconstruction & Inviscid Flux Calculation

To solve the semi-discrete form of the governing Eq. (2.66), the fluxes across the cell faces need to be evaluated. The evaluation of the inviscid fluxes will be covered in this section, followed by a discussion of the viscous flux calculation procedure in the proceeding section.

Inviscid fluxes on the cell faces are calculated after reconstructing a flow state de-



Figure 2.8: Dissection of the hexahedral cell into six tetrahedrons. The faces of the original cell are shaded.



Figure 2.9: Tetrahedron with edge vectors labelled.

scription from the cell-averaged values. The reconstruction process converts known cellaveraged flow properties ( $\rho$ ,  $u_x$ ,  $u_y$ ,  $u_z$ , e, p and  $f_i$ ), into point-wise data located at the middle of each bounding face of the control volume. The accuracy of reconstructing the primitive-variable field at the cell faces determines the spatial accuracy of the solution [226].

### 2.11.1 XFace Inviscid Fluxes

The reconstruction of the flow states on the downwind XFace cell-interfaces (denoted with the subscript  $ix + \frac{1}{2}$ ), is an extrapolation from the cell-averaged values of the previous two upwind upwind cells (i - 2), (i - 1) and the current cell (i) (see Fig. 2.10). The



**Figure 2.10:** Cells used for upwind extrapolation of interface fluxes on the downwind interface  $XFace_{ix+\frac{1}{2}}$ .

extrapolation is done separately for each of the flow variables and species mass fractions, then the estimated flow-field properties are combined to form the cell-interface inviscid fluxes. The fluxes for the upwind  $XFace_{ix-\frac{1}{2}}$  are simply the values from the steady-

state solution of the previous upwind cell. This characteristic-based (upwind) approach is stable for calculating XFace fluxes since the supersonic core flow in the x-direction is hyperbolic and the subsonic regions are treated with pressure splitting making them at least parabolic.

The extrapolation technique used is the Monotone Upstream-centred Scheme for Conservation Laws approach, or MUSCL [226], which is spatially second order accurate. As an example, the downwind cell-interface value for density would be,

$$\rho_{int} = \rho_i + \frac{1}{4} [(1-\kappa)\overline{(\Delta-)}_i + (1+\kappa)\overline{(\Delta+)}_i] \quad , \tag{2.77}$$

where

$$\overline{(\Delta-)}_{i} = \text{MINMOD}(\Delta_{i}, \beta \Delta_{i+1}) ,$$
  
$$\overline{(\Delta+)}_{i} = \text{MINMOD}(\beta \Delta_{i}, \Delta_{i+1}) ,$$
 (2.78)

and

$$\Delta_{i-1} = \rho_{i-1} - \rho_{i-2} ,$$
  

$$\Delta_i = \rho_i - \rho_{i-1} ,$$
  

$$\Delta_{i+1} = \Delta_i + \Delta_i - (\Delta_{i-1}) .$$
(2.79)

The current cell-averaged value is  $\rho_i$ , the next upwind value is  $\rho_{i-1}$  and the next value is  $\rho_{i-2}$  (see Fig. 2.10). The MUSCL scheme used here [16] is slightly modified from the original [226]. The downstream gradient  $\Delta_{i+1}$  is approximated using the two upstream gradients. This limits the accuracy of the scheme to second order. The MUSCL parameter  $\kappa$  is set to -1 making it a fully upwind scheme and the compression parameter for the limiter is set to  $\beta = 2$ .

The minimum modulus (MINMOD) limiter function returns the argument with the minimum magnitude if both arguments have both the same sign and returns zero otherwise. The purpose of the limiter is to maintain stability and eliminate numerical oscillations in regions with large gradients of flow variables. The MINMOD limiter is computationally efficient, but it does not resolve contact discontinuities well and can cause limit cycles in the convergence process. Many other limiters are available and a good treatment of the different types is given in Sweby [214].

Once the fluxes are calculated for the *XFace* cell-interfaces, Vigneron's pressure splitting is applied. The fraction of the pressure that is dropped from the face streamwise momentum term (Eq. 2.9), is determined from the cell-centre flow terms rather than the reconstructed face terms. This is done so that a nonphysical acceleration caused by a variation in  $\varepsilon$  across the cell does not result [156].

### 2.11.2 Inviscid Boundary Conditions

Before the cross-stream fluxes are determined, boundary conditions are applied around the duct walls by setting up a layer of ghost cells (two deep) along each boundary (see Fig. 2.11). The flow properties in the ghost cells are determined from the interior cells



Figure 2.11: Ghost and secondary cells used for the calculation of boundary conditions and viscous derivatives respectively.

and/or the free-stream conditions depending upon the imposed bounding condition. The boundary conditions are updated every iteration in time.

Each of the four walls bounding the flow domain can be set to a different condition. The four walls are denoted *North*, *South*, *East* & *West* which correspond to the top, bottom, right and left walls respectively looking from the inflow plane downstream (for grid corners defined in the order shown in Section 2.14). The boundary conditions that are available are:

- supersonic inflow condition
- solid wall with inviscid (slip) tangency condition
- solid, no-slip, adiabatic wall
- solid, no-slip, fixed temperature wall

When calculating the inviscid fluxes, the inviscid boundary condition is applied, where the velocity vector is found by reflecting the component normal to the cell face (except for a supersonic inflow boundary condition). The first ghost cell to the wall contains the reflected velocity vector from the first interior cell. The second ghost cell contains the reflected velocity vector from the second interior cells. The wall normal is used to find the normal components of the velocity vectors. The temperature, internal energy, pressure, mass fractions and sound speed are all copied from the source cell. A supersonic inflow condition is applied by filling the ghost cells with the specified free-stream quantities. The reconstruction procedure may then be applied (uniformly) across the entire slice irrespective of an interface lying on the domain boundary.

### 2.11.3 Cross-Stream Inviscid Fluxes

The calculation of the cross-stream interface fluxes is a little more involved than the calculation of the streamwise fluxes because there is no dominant (supersonic) flow direction. The cross-stream interfaces,  $iy \pm \frac{1}{2}$  and  $iz \pm \frac{1}{2}$ , require a more robust flux calculation procedure so that oblique shocks within the flow can be captured without large oscillations in the flow properties. Here, a Godunov-type scheme is used which is based on MUSCL reconstruction of the flow properties on the "left" and "right" sides of the interface, followed by the application of an approximate Riemann flux calculator to resolve differences at each of the interfaces. The details of the flux calculator will be covered in the proceeding section.

The generalised MUSCL reconstruction scheme [16] is again applied independently to each of the primary flow variables to give estimates of the flow properties on each side of the cell interfaces. This approach is very similar to the technique used to calculate the fluxes on the XFaces, however, an extrapolation version of MUSCL was used for the XFaces that gave estimates of the interface values directly and was only second-order accurate. For the YFace and ZFaces, a third-order interpolation scheme is used to calculate left and right states. As an example, the density estimates either side of the  $iy + \frac{1}{2}$  interface are

$$\rho_L = \rho_{iy,iz} + \frac{1}{4} \left[ (1-\kappa)\overline{(\Delta-)}_{iy,iz} + (1+\kappa)\overline{(\Delta+)}_{iy,iz} \right] , \qquad (2.80)$$
  

$$\rho_R = \rho_{iy+1,iz} - \frac{1}{4} \left[ (1+\kappa)\overline{(\Delta-)}_{iy+1,iz} + (1-\kappa)\overline{(\Delta+)}_{iy+1,iz} \right] ,$$

where

$$\overline{(\Delta-)}_{iy,iz} = \text{MINMOD}(\Delta_{iy,iz}, \beta \Delta_{iy+1,iz}) , \qquad (2.81)$$
$$\overline{(\Delta+)}_{iy,iz} = \text{MINMOD}(\beta \Delta_{iy,iz}, \Delta_{iy+1,iz}) ,$$
and

$$\Delta_{iy,iz} = \rho_{iy,iz} - \rho_{iy-1,iz} \quad . \tag{2.82}$$

The compression parameter for the limiter is set to  $\beta = 2$  and the spatial accuracy constant is set to  $\kappa = 1/3$ , giving third-order accurate interpolation. Note that the reconstruction is applied independently in the  $\eta$  and  $\zeta$  directions.

In order to apply a one-dimensional flux calculation procedure, the local flow velocities of the interpolated left and right states are rotated into a local frame of reference. In this frame of reference the "local streamwise" direction is aligned with the unit normal for the particular cell interface. This is done by taking the dot product of the velocity with each of the unit vectors associated with the interface

$$u_{n} = u_{x}n_{x} + u_{y}n_{y} + u_{z}n_{z} , \qquad (2.83)$$
  

$$u_{t1} = u_{x}t_{1x} + u_{y}t_{1y} + u_{z}t_{1z} ,$$
  

$$u_{t2} = u_{x}t_{2x} + u_{y}t_{2y} + u_{z}t_{2z} .$$

The normal and tangential velocities of the left and right state are then given to the flux calculator along with the other interpolated flow properties. The interface flow properties estimated by the flux calculator are rotated back to the global Cartesian coordinates using

$$u_{x} = u_{n}n_{x} + u_{t1}t_{1x} + u_{t2}t_{2x} , \qquad (2.84)$$
  

$$u_{y} = u_{n}n_{y} + u_{t1}t_{1y} + u_{t2}t_{2y} , \qquad u_{z} = u_{n}n_{z} + u_{t1}t_{1z} + u_{t2}t_{2z} ,$$

and then combined to form the inviscid flux components of Eq. (2.66).

#### 2.11.4 Approximate Riemann Flux Calculator

The cross-stream inviscid fluxes between cells are calculated using the Osher type upwind approximate Riemann solver of Jacobs [107] and the efficient linearized flux solver of Toro [223]. Regions of slowly varying data are solved using Toro's linearized solver [223] since it requires very few computational calculations and produces reasonable results in regions of applicability. For the remainder of the flow domain, an implementation of Jacobs' approximate flux calculator [107] is used without the strong-shock stage. Jacobs' solver is very similar to Osher's robust approximate Riemann solver [167], and it has been shown to be accurate in inviscid and viscous flows [105, 109]. It has the ability to capture shock waves and other sharp features with optimal resolution and with reduced spurious oscillations of traditional finite-difference methods with artificial viscosity. Its conservative character ensures correct positions of the computed shock waves and its robustness ensures good stability in high gradient flow situations. When used in conjunction with Toro's linearized solver, a computationally efficient scheme results that retains the robustness of Osher's solver.

The implementation of the solver scheme is broken up into two stages. First, the intermediate states between the left and right running waves are calculated, then the interface state is selected or interpolated from the intermediate states and the left and right states. Toro's solver [223] is used initially in the first stage to calculate the pressure and the velocity in the intermediate region. The applicability of Toro's solver can then be determined from the intermediate states. The intermediate region and Toro's solution can be described as follows.

The Riemann problem solution can be considered to contain four constant states separated by three waves as shown in Fig. 2.12. The left and right running waves can either



**Figure 2.12:** Structure of the exact solution to the Riemann problem for the time-dependent, onedimensional Euler equations (U represents the state vector).

be shocks or rarefactions and the middle wave is always a contact discontinuity. Toro's linearized solver solves approximately for the intermediate region between the left and right waves denoted as the star region, where the pressure and velocity remain constant and the density undergoes a change across the contact. The solution proposed by Toro is,

$$u^* = \frac{1}{2}(u_L + u_R) - (p_R - p_L)/(2\bar{\rho}\bar{a})$$
(2.85)

$$p^* = \frac{1}{2}(p_L + p_R) - \frac{1}{2}\bar{\rho}\bar{a}(u_R - u_L)$$
(2.86)

$$\rho_L^* = \rho_L + (u_L - u^*)\bar{\rho}/\bar{a}$$
(2.87)

$$\rho_R^* = \rho_R + (u^* - u_R)\bar{\rho}/\bar{a} \quad , \tag{2.88}$$

where the average density and sound speed between the left and right state is given as,

$$\bar{\rho} = (\rho_L \rho_R)^{\frac{1}{2}}$$
, and  $\bar{a} = \frac{1}{2}(a_L + a_R)$ . (2.89)

A beneficial feature of the solution proposed by Toro is that for the case of an isolated contact discontinuity travelling with speed  $u^* = u_L = u_R$  the solution is exact.

The linearized solver of Toro is intended to only be used in regions of slowly varying data. The suggested criteria for the application of the solver is,

$$p_{\min} \le p^* \le p_{\max} \tag{2.90}$$

$$-p_{\min} \le \bar{\rho}\bar{a}(u_L - u_R) \le p_{\min} \quad , \tag{2.91}$$

where  $p_{\min}$  and  $p_{\max}$  are the minimum and maximum of  $p_L$  and  $p_R$ . This ensures that the solver is never applied to cases where (a) the left and right moving waves are both rarefactions or shocks, and (b) the pressure ratio across the left and right state exceeds 2.

The criteria for applying Toro's solution can be checked after the intermediate pressure and velocity are calculated  $(p^*, u^*)$ . If it is applicable, the rest of the intermediate flow variables are calculated. If not, Jacobs' solver [107] is applied to calculate the intermediate flow variables. Once the intermediate states are calculated, the position of the interface state in relation to the Riemann solution is determined. The position of the interface is essentially determined from the wave speeds of the left and right waves. If the interface is found to straddle an expansion fan, linear interpolation is used to calculate the flow velocity and then the isentropic relations are used to calculate the remaining flow properties [134].

When implementing the flux solver for chemically reacting flows, the chemistry is assumed to be frozen as the flow variables are convected across the interface. Jacobs' solver [107] is modified for chemically reacting flow where a difference in  $\gamma$  occurs across the interface by using a Roe averaged  $\gamma$  for calculating the Riemann invariants [68]. The Osher solver [167], on which Jacobs' solver is based, was derived for an ideal nonreacting gas and as a result produces small oscillations in the solution variables in regions of concentration gradients [57]. By using a Roe averaged  $\gamma$ ,

$$\bar{\gamma}_{\rm av} = \frac{\sqrt{\rho_L \gamma_L} + \sqrt{\rho_R \gamma_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad , \tag{2.92}$$

when calculating the Riemann invariants, the magnitude of the oscillations can be reduced to a magnitude of less than 1% of the nominal value of the variables [57].

The mass fluxes of the species are constructed from the calculated cell interface velocity and the species densities from the left or right cell centres. If the interface velocity is positive, the species fluxes are composed of the species densities on the left side of the interface. For negative velocities, the species densities on the right side of the interface are used.

#### 2.12 Calculating the Viscous Fluxes

The viscous fluxes are calculated from numerical approximations of the velocity and temperature derivatives in Eqs. (2.7) and (2.8). The transport coefficients also need to be calculated, however, they can be determined from functions of the explicitly specified gas state at the interfaces and domain boundaries.

The divergence theorem is used to calculate the derivatives at cell vertices. The derivatives at each of the four vertices making up each cell face are then averaged to get the interface derivative. The divergence theorem can be written as

$$\frac{1}{V} \int_{V} \nabla \phi \, dV = \frac{1}{V} \oint (\phi \, \hat{n}) dA \quad , \tag{2.93}$$

where  $\phi$  represents some arbitrary scalar variable.

The divergence theorem can be used to calculate viscous derivatives at cell vertices by forming secondary cells around each vertex. The secondary cells provide a control volume for which the divergence theorem can be explicitly applied. The cell centres of the current, upwind and downwind primary cells, form the vertices of two slices of secondary cells (see Fig. 2.11). Therefore, for each primary cell, four upstream and four downstream secondary cells need to be formed. The flow properties  $u_x$ ,  $u_y$ ,  $u_z$  and T at the cell centres of the primary cells are copied to the vertices of the secondary cells and the areas, volumes and unit normals on the faces of the secondary cells are then calculated. The vertices of secondary cells on the boundaries of the computational domain are constructed using the primary cell centres of the cells nearest to the boundary and the centres of the cell faces that form the boundaries. These cells constitutes a half cell; similarly, corner secondary cells are quarter cells.

The semi-discrete form of the divergence theorem can be applied to the secondary cells as

$$\left(\frac{\partial\phi}{\partial x}\right)_{i,j} = \frac{1}{4} \frac{1}{V_{i,j}} \sum_{i=\text{face } 1}^{\text{face } 6} A_i(\hat{\mathbf{n}}_i.\hat{\mathbf{i}})(\phi^1 + \phi^2 + \phi^3 + \phi^4) , \qquad (2.94)$$

$$\left(\frac{\partial\phi}{\partial y}\right)_{i,j} = \frac{1}{4} \frac{1}{V_{i,j}} \sum_{i=\text{face } 1}^{\text{face } 6} A_i(\hat{\mathbf{n}}_i.\hat{\mathbf{j}})(\phi^1 + \phi^2 + \phi^3 + \phi^4) ,$$

$$\left(\frac{\partial\phi}{\partial z}\right)_{i,j} = \frac{1}{4} \frac{1}{V_{i,j}} \sum_{i=\text{face } 1}^{\text{face } 6} A_i(\hat{\mathbf{n}}_i.\hat{\mathbf{k}})(\phi^1 + \phi^2 + \phi^3 + \phi^4) ,$$

$$(2.95)$$

where  $V_{i,j}$  is the volume of the secondary cell, faces 1 to 6 are the six faces of the secondary cell, and  $\phi^1, \phi^2, \phi^3, \phi^4$  are the flow variables at the four vertices of each secondary

cell face. The derivatives evaluated at the centres of the secondary cells are then copied to the primary cell vertices. The four vertex values making up each cell face are then averaged to get the derivative values at the primary cell interfaces.

#### 2.12.1 Viscous Boundary Conditions

Viscous derivatives and transport coefficients are calculated at the computational domain boundaries by applying viscous boundary conditions. Boundary conditions are applied by setting the flow properties at the cell interfaces that form the domain boundaries. When the boundary conditions are set to solid, no-slip, adiabatic or isothermal walls, all the velocity components are set to zero at the boundary interfaces. Isothermal or adiabatic wall conditions can be set by maintaining a fixed temperature on the boundary interfaces for isothermal conditions or by setting the temperature to the adjacent primary cell centred value for adiabatic conditions.

If a solid wall with an inviscid tangency condition is selected, cell-centred values of the first inviscid ghost cell and the first adjacent interior cell are averaged to form the boundary interface values. This condition would be set for a plane of symmetry.

A viscous supersonic inflow condition is the same as the inviscid condition where the boundary interface flow properties are set to the free-stream values.

### 2.13 Time Integration for Each Slice

The simplest way of integrating the governing equations is to use an explicit time-stepping scheme. Once the time differentials of dependent flow variables for each cell in the slice are obtained from Eq. (2.66), the solution is stepped forward in time by a small amount  $\Delta t$  by applying the scheme

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \, \frac{d\mathbf{U}^n}{dt} \quad . \tag{2.96}$$

This simple scheme is used in preference of more elaborate predictor-corrector and implicit schemes. The latter schemes require increased computational effort which is an important consideration for large three-dimensional problems. The explicit scheme is also simple to code and requires less data storage than implicit methods. However, this approach is not as robust as implicit schemes so time steps have to be restricted to maintain stability.

The time integration of the flux terms and chemical source terms in the governing equation, Eq. (2.1), are coupled in an approximate manner to simplify the scheme. The species production terms in the source term vector are calculated for the flow conditions

at time n. The flux terms are also calculated for the flow conditions at time n assuming frozen flow. The conserved flow variables are then stepped forward in time to n + 1using the explicit scheme in Eq. (2.96). After updating the species mass fractions (due to both convection and production), cell density and internal energy at the time level n + 1, the new temperature is calculated using an iterative secant method (see Section 2.6.2). Once the temperature is obtained, the pressure and sound speed can be calculated from the equation of state. The integration process then starts again for the next time step. This integration approach is similar to that used by Wadawadigi *et al.* [232]. An advantage of this scheme is that the size of the chemistry model does not have any effect on the integration procedure unlike implicit schemes which become computationally intensive when performing large block inversions due to numerous chemical species.

The time step  $\Delta t$  in the explicit scheme, is a functions of the smallest time scale present in the solution slice.

$$\Delta t = \text{CFL} \quad \cdot \quad \text{MIN} \left( \Delta t_{\xi}, \ \Delta t_{\eta}, \ \Delta t_{\zeta}, \ \Delta t_{\text{viscous}}, \ \Delta t_{\text{chem}} \right)$$
(2.97)

There are three inviscid acoustic time scales, a viscous time scale and a time scale based on the fastest reaction rate. The three acoustic time scales are approximate times for acoustic waves to travel through a cell in each each of the three coordinates,  $(\xi, \eta, \zeta)$ .

$$\Delta t_{\xi} = \frac{u_x + a}{L_{\xi}}$$

$$\Delta t_{\eta} = \frac{u_{\max \text{ ws, YFace}}}{L_{\eta}}$$

$$\Delta t_{\zeta} = \frac{u_{\max \text{ ws, ZFace}}}{L_{\zeta}}$$
(2.98)

The wave speed used in the time scale,  $\Delta t_{\xi}$ , is calculated by summing the component of velocity in the x direction and the sound speed that has been reconstructed on the downwind XFace. The other two inviscid time scales in the cross-stream directions, use the maximum wave speed at each cell face returned by the flux calculator. The characteristic length scales  $(L_{\xi}, L_{\eta} \text{ and } L_{\zeta})$  are approximate distances from respective centres of opposing cell faces. The viscous time scale [213] is approximated as

$$\Delta t_{\rm viscous} = \frac{Pr\,\rho}{4\mu\gamma} \left(\frac{1}{L_{\xi}^2} + \frac{1}{L_{\eta}^2} + \frac{1}{L_{\zeta}^2}\right)^{-1} \quad . \tag{2.99}$$

Stability of chemical reactions in the time integration is maintained by limiting the time step with a chemical time scale. The chemical time scale is selected such that no change in species density  $(\rho f_i)$  greater than  $1 \times 10^{-4} \text{ kg/m}^3$  occurs over a time step. The

chemical time scale is written as

$$\Delta t_{\rm chem} = \frac{1 \times 10^{-4} \text{ kg/m}^3}{\dot{\omega}_{\rm max}} \quad . \tag{2.100}$$

The chemical time scale can be significantly smaller than the inviscid and viscous time scales when computing reacting flows. This disparity in time scales is known as stiffness and results in very small time steps for maintaining stability. Stiffness can be overcome by using implicit techniques (such as a point implicit algorithm for the species transport equations [117]) however this adds complexity to the code. The approach taken in sm3d is to forgo the use of an implicit technique since the solver is thought to be fast enough to make the use of the chemical time scale practical.

The CFL value is the "Courant-Friedrichs-Lewy number" which is a number obtained from a Von Neumann stability analysis of the scaler wave equations. A limit on the value of the CFL number is obtained from reference [38] as

$$CFL \le \frac{4}{5 - \kappa + \beta(1 + \kappa)} \quad . \tag{2.101}$$

With  $\kappa = 1/3$  and  $\beta = 2$ , the upper limit for CFL is 0.55, however, because we cannot always make good estimates of the wave speeds across all cells, a value of CFL = 0.25 is suggested. In cases where the cells become highly elongated (such as circular duct cross-sections), a smaller value may be appropriate.

The governing equations are integrated in time using the scheme in Eq. (2.96) until the whole slice has reached a steady state. The following criteria are checked after each time step to confirm a steady state condition:

- Relative changes in density over a time step are less than a specified tolerance (typically 10<sup>-4</sup>).
- At least five flow lengths have passed through the cell that contained the smallest time scale. If the flow speed is subsonic in the ξ direction for the determining cell, the sound speed is used to calculate the time for a flow length to pass.
- A maximum number of time steps has not been exceeded (typically 100 for non-reacting and 500 for reacting flows).

Once a steady-state solution is obtained for the current slice, the solver cycles through the data structures maintaining the data for the last two slices for extrapolation, and then proceeds to work on the next downwind slice.

### 2.14 Grid Generation

The computational domain is discretized using a structured grid composed of slices of hexahedral cells. A schematic of the hexahedral discretization is shown in Fig. 2.13. The "bounding box" that contains the slices can be specified using simple straight edge



Figure 2.13: Grid formulation for the space-marching solver.

panels, panels whose edges are defined by Bézier curves or B-spline surfaces. Examples of these different types of bounding box are shown in Fig. 2.14. Straight edge panel grids are defined by a set of (x, y, z) position data that specifies the corner points of each panel making up the grid. Similarly, a set of (x, y, z) position data specify Bézier control points for the lines making up the streamwise edges of the Bézier panels. An *n*th degree Bézier polynomial determined by n + 1 control points is given by

$$p(\xi) = \sum_{i=0}^{n} \binom{n}{i} (1-\xi)^{n-1} \xi^{i} p_{i}, \quad \text{where} \qquad (2.102)$$
$$\binom{n}{i} = \frac{n!}{i!(n-i)!}.$$

The parametric  $\xi$  coordinate ranges from 0 to 1 and determines the position along the Bézier polynomial.

A segment of a straight edged bounding box is shown in Fig. 2.15 with the corner points labelled. The straight edge panels are made up of linearly interpolated surfaces between neighbouring points where the lines (A'A), (B'B), (C'C), and (D'D) specify the locations of corner points for each vertex slice. For any  $\xi$  value, the corner points are located on these lines using linear interpolation. These points are then joined to form the bounds of the slice. Bézier grids are created in a similar fashion, except for the lines specifying the locations of vertex slice corner points which are replaced with Bézier curves.



**Figure 2.14:** Examples of grid bounding boxes that can be generated by the solver; *top:* straight edge panels, *middle:* panels with  $\xi$ -edges defined by Bézier curves, *bottom:* B-spline surfaces forming the  $\eta - \zeta$  exterior surfaces.

B-spline surfaces are used for more complex contoured geometries where the boundaries, of each vertex slice are curved. B-spline surfaces are made from four control net data files which are generated from the suite of programs in [44].

Once the edges of the constant  $\xi$  slices are defined using any of the three methods described, an array of vertices in the  $(\eta, \zeta)$ -plane is generated as shown in Fig. 2.16. The vertices are generated from a set of parameterised interpolation points  $\overline{P}_{DA}(\zeta)$ ,  $\overline{P}_{CB}(\zeta)$ ,  $\overline{P}_{DC}(\eta)$ , and  $\overline{P}_{AB}(\eta)$  for  $0 \le \eta \le 1$  and  $0 \le \zeta \le 1$ . Transfinite interpolation (or a Coons patch [182]) is then used to obtain the position of the vertex as

$$\overline{P} = (1-\eta)\overline{P}_{DA} + \eta\overline{P}_{CB} + (1-\zeta)\overline{P}_{DC} + \zeta\overline{P}_{AB}$$

$$-(1-\eta)(1-\zeta)\overline{P}_{D} - (1-\eta)\zeta\overline{P}_{A} - \eta(1-\zeta)\overline{P}_{C} - \eta\zeta\overline{P}_{B} ,$$

$$(2.103)$$



Figure 2.15: Exterior surfaces of the grid bounding box and defining corner points.



**Figure 2.16:** Transfinite patch interpolation in the  $(\eta, \zeta)$ -plane.

where  $\overline{P}_A$  to  $\overline{P}_D$  are the positions of the corners of the vertex slice. Once a slice of vertex points has been constructed, a small step is taken in  $\xi$  to generate another downstream slice of vertex points. These two vertex slices form the corner points of the hexahedral cells.

Even though a structured hexahedral discretization is used in sm3d, the six sided bounding box can be fitted to many types of geometries since the interpolation points and corner points need not be coplanar in the Cartesian coordinate system. Also, the corners of the  $\xi$  slices need not be corners in a physical sense. For example, a circle in the Cartesian coordinate system may be mapped to a square in the  $(\eta, \zeta)$ -plane as in Fig. 2.17. The bounding box can also be wrapped around bodies such as cones and cylinders making it suitable for external flow modelling. An example of a grid for a cone is given in Fig. 2.18. The grid shown is composed of grid points at every twentieth axial plane to improve clarity. The space-marching solution scheme assumes that there is little change in flow properties between neighboring cells in the space marching direction. Consequently, small step sizes are used in the space marching direction to maintain numerical stability. This approach results in computational cells with large aspect ratios (i.e. very



**Figure 2.17:** Example of a cross-stream grid for a duct with circular cross-section (quarter sector shown).

thin in the streamwise direction), particularly for cells far from boundary layers in viscous cases where the grid is clustered towards the wall. The optimum spacing between space-marching slices for each simulation is determined by trial and error.

Grids for two-dimensional and axisymmetric cases can be constructed using straight edge or Bézier bounding boxes that are two cells wide in the  $\zeta$  direction. The (x, y)coordinate data are specified for the corner points of each bounding box segment and the z coordinates are set by the code. The bounding box in made 2 metres thick in the z direction so that each cell is 1 metre wide. During the computation, all fluxes in the z direction are set to zero and calculations are limited to the first plane of cells in this direction for computational efficiency.

The interpolation points used in the transfinite interpolation (Eq. (2.103)) can be clustered using a Roberts stretching function [5]. The clustering technique uses an exponential formula to cluster parametric points either to one side or both. For a given parametric point  $\eta$ , the clustered point  $\bar{\eta}$  would be

$$\bar{\eta} = \frac{\left(\beta + 2\alpha\right) \left(\frac{\beta+1}{\beta-1}\right)^{\left(\frac{\eta-\alpha}{1-\alpha}\right)} - \beta + 2\alpha}{\left(2\alpha + 1\right) \left(1 + \left(\frac{\beta+1}{\beta-1}\right)^{\left(\frac{\eta-\alpha}{1-\alpha}\right)}\right)} \quad , \tag{2.104}$$

where  $\beta$  is the clustering parameter and  $\alpha$  determines the position of the clustering. The range of the clustering parameter is  $(1 < \beta < +\infty)$  where the closer  $\beta$  is to 1, the greater the clustering. If  $\alpha$  is equal to 0.0, the points will be clustered to the end where  $\eta = 1$ . If  $\alpha$  is equal to 0.5, the points will be clustered at both extremes.



Figure 2.18: Example grid for flow over a cone.

The clustering function in Eq. (2.104) permits clustering at both ends of a parametric range however the clustering level at the  $\eta = 0$  end is dependent on the value of  $\beta$  and can't be set independently. Korte & Hodge [123] proposed a method of blending two clustering functions using a fourth order polynomial to give greater control of the clustering levels at each end of a parametric range. A clustering parameter can be specified for each end, however, the fourth order polynomial still tends to weight the function to one end. A more centred approach is to use a trigonometric term to blend the two functions. The proposed blending transformation is given by

$$\bar{\eta} = (1 - \chi) \left( 1 - \beta_0 + \frac{2\beta_0}{1 + \left(\frac{\beta_0 + 1}{\beta_0 - 1}\right)^{1 - \eta}} \right) + \chi \left( \beta_1 - \frac{2\beta_1}{1 + \left(\frac{\beta_1 + 1}{\beta_1 - 1}\right)^{\eta}} \right)$$
(2.105)

where

$$\chi = \frac{\left(\sin\left(|\pi(\eta - \frac{1}{2})|\right)\right)^{\frac{1}{3}} + 1}{2} \cdot \frac{\eta - \frac{1}{2}}{|\eta - \frac{1}{2}|}$$
(2.106)

The coefficient  $\beta_0$  is the clustering parameter for the points closest to  $\eta = 0$  and  $\beta_1$  is the clustering parameter for the points closest to  $\eta = 1$ . The cube root sine term in Eq. (2.106) effectively provides a smooth switching term between the two clustering functions.

A third clustering transformation was also implemented which clusters a distribution of parametric points,  $\eta$ , about some internal point,  $\eta_c$ . This clustering transformation [220] can be expressed as

$$\bar{\eta} = \eta_c \left( 1 + \frac{\sinh[\beta(\eta - A)]}{\sinh(\beta A)} \right)$$
(2.107)

where

$$A = \frac{1}{2\beta} \ln \left[ \frac{1 + (e^{\beta} - 1)\eta}{1 + (e^{-\beta} - 1)\eta} \right]$$

The transformed parametric point is  $\bar{\eta}$  and the clustering parameter is  $\beta$  which ranges from 0 for no clustering, to  $\infty$  for infinite clustering.

#### 2.15 Further Remarks on the Flow Solver

The PNS flow solver discussed in this chapter was used to solve a number of test case problems in Appendix E. The solutions to these problems demonstrate the solver's ability to accurately apply the implemented phenomenological models by comparing well with experimental results and other published works. Execution times are also provided, which serve to demonstrate the solver's computational speed. Operational details for the solver are provided in a separate document [45] and have been omitted for brevity. The complete flow simulation software package and operational details are available on CD-ROM on request through The Department of Mechanical Engineering at The University of Queensland.

A large part of the time devoted to this thesis was spent developing the code for the flow solver. The flow solver code is like many other research codes that implement published models, algorithms and techniques in a new and original way. Also, like other research codes, many of the capabilities of the code are matched by commercial codes that are readily available and could have completed the flow simulations contained within this thesis. However, there are several reasons why the code was written rather than using an existing code.

Firstly, writing the code was a valuable experience that trained the author in CFD techniques that would otherwise not have been obtained through the use of a "black box" type flow solver or commercial package. CFD is still an evolving science that requires a thorough knowledge of the principles and theory behind it in order to use it in a practical and effective way.

Secondly, having access to, and knowledge of, the source code was instrumental in maximising the performance of the code for the design problems addressed. Compu-

tational design optimization requires many flow calculations to be performed rapidly to make the design method practical. By using a commercial code, the user is limited to the performance of the code as it is supplied and it cannot be easily tailored for a particular class of flow problems. Having access to the source code also removed difficulties with incorporating an optimization algorithm.

Lastly, the flow solver adds to the capabilities of the suite of CFD solvers that have been developed in The Department of Mechanical Engineering at The University of Queensland, which are actively used by researchers and students alike to further knowledge in the area of compressible fluid mechanics.

# **Design Optimization**

The previous chapter described a compressible three-dimensional flow solver that could be used to provide the data for evaluating the objective function in a design optimization problem. This chapter is concerned with the optimization algorithm itself. The chapter starts with a brief overview of the common classes of optimization algorithms used for aerodynamic design. Then, a detailed description of the optimization algorithm selected for use in this study is given, followed by a discussion of how the flow solver and optimization algorithm were coupled together to form the design tool. Finally, a literature review of some of the more recent applications of optimization in the fields of scramjet design and nozzle design is presented. The review provides useful insights on how to apply computational optimization to the design problems presented in chapters 4, 5 and 7.

## 3.1 Optimization Algorithms

Optimization algorithms coupled with flow solvers have been used for a number of aerodynamic design problems. Some examples of recent applications are airfoils with high lift to drag ratios [66, 59, 130], three-dimensional hypersonic lifting bodies [65], turbofan engines [94], hypersonic wind tunnel nozzles [125, 118, 222] and scramjet vehicles designed for maximum axial thrust [22, 148, 191]. Most of the cited examples employ one of two types (or classes) of optimization algorithms, which use different approaches to determine a function's minimum point. These two classes of algorithms are: (i) gradient-search algorithms; and (ii) genetic algorithms (GA), which are non-gradient, stochastic methods [93, 71, 53]. The gradient-search class can be broken down further into two smaller classes, which are design-variable sensitivity formulations [193] and simplex minimisation [200, 159, 164].

Gradient-search algorithms based on design-variable sensitivities have been used in studies conducted by Korte *et. al* [125], McQuade *et. al* [148] and Sabean & Lewis [191]. The sensitivity approach requires the evaluation of derivatives that quantify the sensitivity of the objective function to the change in each design-variable at a given point in the design space. A matrix of the evaluated sensitivities is constructed and then in-

verted to solve for a search direction for the minimum of the objective function<sup>1</sup>. After a move is made, the sensitivity matrix is updated. Some methods that have been used to invert the sensitivity matrix are the least-squares method [97], Gaussian elimination [145], and a quasi-Newton method [191]. Sensitivity-based optimization algorithms generally converge to an optimum design with fewer iterations compared to other optimization algorithms. When estimating the gradient, however, the algorithms can require a high number of flow solutions to be computed per iteration, particularly for problems with large vectors of design variables. Another limitation of sensitivity-based optimization algorithms is the requirement of a continuously differentiable design space. This may not be the case for high speed compressible flows with embedded shocks.

An extension to sensitivity-based optimization was made by the group of Baysal, Eleshaky & Burgreen [22, 23, 34]. They devised an efficient sensitivity-based optimization scheme and applied it to the design of wing profiles and simplified scramjet-afterbody configurations. The efficiency of the scheme is a result of using a quasi-analytical method to compute the sensitivity derivatives, rather than the more traditional method of using finite-differences that are evaluated from many computationally intensive CFD flow calculations. Baysal et. al also increased search efficiency by performing short searches along directions determined by the optimizer, with an approximate flow analysis to obtain flow-field solutions and objective functions, rather than solving the complete Euler or Navier-Stokes equations. This approach has also been adopted by McQuade et al. [148] to optimize the surfaces of a two-dimensional scramjet vehicle flow path. Having found a minimum along the search direction, a complete flow solution is computed by the flow solver, and the sensitivity coefficients are evaluated again. The search algorithm is repeated until the optimum design solution is found. This approach to optimization has been shown to be effective, however, the extension of the method to the design of aerodynamic bodies that require modelling of viscous and chemically reacting flows, has not been achieved to date due to the complexities associated with the quasi-analytical method for calculating sensitivities. The method used for calculating sensitivities is also problem dependent, which makes adaptation of the optimization method to different design problems a non-trivial exercise.

Simplex minimisation is similar to sensitivity-based techniques in that the search direction is based on the gradient of the design space. However, simplex minimisation is a "direct" method that does not require the evaluation of derivatives to determine a search direction. Therefore, it is readily applicable to problems that are analytically difficult [164]. The search direction is determined from the objective function evaluations of a "simplex". An initial simplex is formed with (n + 1) vertices, where n is the number of

<sup>&</sup>lt;sup>1</sup>The phrases *finding the minimum of the objective function* and *optimization* essentially have the same meaning and will be used interchangeably.

#### 3.1 Optimization Algorithms

design variables. The first vertex of the simplex is the objective function evaluation for an initial vector of design variables. The remaining n vertices are formed by individually perturbing each design-variable a small amount and evaluating the objective function. An example of a two variable initial simplex is shown in Fig. 3.1, where  $x_1$  and  $x_2$  are the design variables and the objective function evaluates to y. Once the initial simplex is



Figure 3.1: Diagrammatic representation of a two variable initial simplex.

established, movement is then made away from the vertex with the poorest (or highest) objective function evaluation in order to find a replacement for it. Spendley *et al.* [200] introduced this idea and it was later improved upon by Nelder & Mead [159]. Nelder & Mead made the process adaptive, whereby the simplex is continually revised to conform to the nature of the design space (or response surface). The simplex then contracts to the final minimum. Further modifications were made by Routh *et al.* [185] and Parker *et al.* [170], where a curve was fitted to the search direction to find the optimum distance to move in the search space. This modification makes the algorithm slightly more complicated than the algorithm for the Nelder & Mead method, but offers better convergence on relatively simple response surfaces.

Gradient-search techniques generally have good convergence characteristics, however, they are susceptible to convergence about local minima rather than the global minimum. Design spaces that do not have a well defined global minimum point require a "good guess" of the initial design vector close to the global minimum. If this is not possible, multiple optimization problems have to be solved with initial design vectors spanning the design space in order to find the global minimum.

Genetic Algorithms (GAs) represent a class of adaptive algorithms whose search methods are based on the simulation of natural selection and genetics [92]. A GA performs a multi-directional search by maintaining a population of potential solutions and encouraging information formation and exchange between these directions. The population of each generation undergoes a simulated evolution where the relatively "good" solutions reproduce, while the relatively "bad" solutions die. GAs show good exploration of the design space and tend to avoid local minima [162], however, convergence rates are poor in a localised search space [149] and they require large amounts of computational time to maintain population levels [65]. A comprehensive overview of GAs is presented by Goldberg [71].

As outlined above, there are advantages and disadvantages associated with each class of optimization algorithm, which make them applicable to some aerodynamic design problems and not others. However, a recent study conducted by Salomon [192] indicated that GAs and other stochastic methods are generally not as efficient as gradient methods when considering an equal distribution of all possible objective functions. That being said, GAs are superior in searching entire design spaces. In order to make use of the qualities associated with both non-gradient and gradient-search algorithms, one could develop a hybrid algorithm, however, it would not necessarily be the most efficient technique.

An emphasis of computational efficiency and simplicity was placed on the current study, hence, the idea of a hybrid optimization algorithm was not explored. Rather, the simple and robust simplex gradient-search algorithm of Nelder & Mead [159] was employed as the optimization algorithm of choice. A gradient-search algorithm was used in preference to a GA for two reasons. Firstly, the design problems that were considered in the present study were expected to not have a particularly large design space. Reasonably small vectors of design variables were used in design spaces that were confined by structural and manufacturing constraints. Secondly, the design of the scramjet engine required the CFD flow solver to include finite-rate chemical kinetic effects. As a consequence, the computational time required for each flow solution was substantial. GAs can become impractical for these types of design problems because of the large number of objective function evaluations required to find a global minimum. Also, the difficulty of evaluating analytical design solutions for a chemically reacting, viscous flow excluded the use of a quasi-analytical, sensitivity-based optimization algorithm.

## 3.2 Nelder-Mead Optimization Algorithm

As mentioned earlier, the simplex optimization algorithm of Nelder & Mead [159] is based on the original simplex idea of Spendley *et al.* [200]. Nelder & Mead improved Spendley *et al.*'s method by making the simplex capable of adapting itself to the local topography of the design space, such that (in a two-dimensional sense) it elongates down long inclined planes, changes direction on encountering a valley at an angle, and contracts in the neighbourhood of a minimum. Therefore, the perturbation values used to form the initial simplex from the initial design vector are (generally) not critical to the success of the algorithm for design spaces possessing a well defined global minimum.

The algorithm itself is simple and easy to code in comparison to more complex sensitivity-based optimization algorithms. It can be applied to wide variety of optimization problems with relative ease since it does not have any special requirements of the design space other than it be continuous, but not necessarily continuously differentiable. The simplicity of the algorithm comes at a cost of not performing well in regions of stable, slowly varying design spaces. The movement of the simplex is based on clear and perceptible differences between objective function evaluations at each simplex vertex. Therefore, the simplex movement becomes somewhat inefficient in stable regions. Also, several optimization attempts with different initial design vectors may be required to accurately evaluate the global minimum.

The principle of the Nelder & Mead simplex minimisation algorithm can be described by considering an objective function of n variables that is to be minimised. The algorithm starts by forming a simplex in n-dimensional space, where the simplex is a set of (n + 1)function evaluations with each evaluation having a different set of design variables. The best and worst function evaluations of the simplex are identified and a move is made away from the worst evaluation (where the worst evaluation has the highest value). This move may be in the form of a reflection, contraction, or shrinkage depending on the characteristics of the response surface. These movements give the algorithm its adaptive behaviour.

As an example, consider a two-dimensional case where the objective function to be minimised is a function of two variables,  $x_1$  and  $x_2$ . A simplex, **ABC**, is formed as illustrated in Fig. 3.2, where each point represents an evaluation of the function to be minimised. Contours of the objective function are shown as dotted lines. If **A** represents the highest function evaluation, then a reflection is made through the centroid or average



Figure 3.2: Two-Dimensional Simplex.

of the remaining points, which for this two-dimensional case is the bisection point B' of the line joining B and C. The scale of the reflected segment, B'E, is selected by the user. However, a recommended reflection scale is 1:1 [159]. The extension and contraction scales are also recommended to be set to 1:2 and 1:0.5, respectively [159]. If the evaluation of the objective function at the reflected point E results in a lower value than the remaining simplex points, then an extension to point F would ensue. The resulting simplex would then be BCF. The movement of the simplex would then continue with a reflection of the highest objective function evaluation through the centroid of the remaining points. The complete list of possible actions following the evaluation of point E are given in Table 3.1. These actions would continue until the evaluated objective function

**Table 3.1:** Conditions governing the formation of subsequent simplexes.

Condition	Action	New Simplex
$f(C) \le f(E) \le f(B)$		BCE
f(E) < f(C)	Extend	BCF
f(A) < f(E)	Contract	BCG
$f(B) < f(E) \le f(A)$	Contract	BCH
$f(A) \le f(G) \text{ or } f(E) \le f(H)$	Shrink	A'B'C

value for the new point was between the lowest and the highest value of the original simplex (first condition in the table). The simplex movement would then start again with a centred reflection.

The simplex moves through the design space searching for a minimum until one of two conditions is reached: (a) the value of the smallest objective function evaluation is less than a prescribed goal, or (b) the variation in objective function evaluations at each simplex vertex is less than a prescribed value. The variation in objective function values is quantified by calculating the variance, s, as

$$s = \sqrt{\frac{1}{n} \sum_{1}^{n+1} (y_i - \bar{y})^2} \quad , \tag{3.1}$$

where  $y_i$  are the evaluations of the objective functions at each vertex point in the simplex and n is the number of design variables. This criterion for convergence is effective as long as the simplex does not become too small in relation to the slope of the design surface prior to reaching the minimum.

Movement of the simplex in the design space can be constrained to exclude unwanted design solutions by using one of two techniques. The objective function can be set to a

very high number when a design-variable goes outside its bounds. This represents the socalled method of "external penalties". Any movement of the simplex outside the bounds of a design-variable results in an automatic contraction of the simplex that will eventually keep it within the boundaries. Alternatively, if the constraint for a design-variable is that it must always maintain a positive value, then the scale of the variable can be transformed (for example by using the logarithm) so that negative values are excluded. A limitation of both these methods is that minima on the boundary of the design space are excluded from the search, however, arbitrarily close approaches to the boundary can be made.

#### **3.3 Implementation and Coupling to the Flow Solver**

The coding of the Nelder & Mead optimization algorithm was based on a "C" translation of a "FORTRAN" code presented by O'Neill [165]. The code of the optimization algorithm was written as a separate function that is called by a main program. Within the main program is a library of initial design-variable vectors and associated initial perturbations for each design case. Upon starting the main program and specifying the case to be solved, the program identifies the initial design-variable vector and proceeds to construct a simplex using the given design-variable perturbations. For each design vector (or vertex) making up the simplex, the program calls the flow solver which returns the flow solution associated with the given design vector. The main program uses the flow solution data to evaluate the objective function and then passes this information to the optimizer. The optimizer then returns instructions on how to move the simplex.

The variables that make up the design vector are used by the flow solver to specify the geometry of a flow domain. Examples of variables that may be used are the coordinates of Bézier curve control points, coordinates of domain corners, increments in distances between subsequent computational cells along a duct, control points of B-Spline surfaces, or scaling parameters for a group of points defining the boundary of the domain. The goal when selecting the design variables is to have as few as possible and have them strongly coupled to the objective function [124].

The objective function typically quantifies a deviation of some flow variable or force from a target value. An example of an objective function for shock tunnel nozzles might be a function that expresses the variation of Mach number and flow angularity at selected points within the flow-field. Other quantities of variation for scramjet design may be deviations from a desired thrust or specific impulse, total drag on a body, or mass fractions of unburnt fuel species. Typically, the objective function is formulated so that the desired design is achieved when the objective function evaluates to the global minimum. It is important to formulate the objective function so that there is a clear minimum point in the design space. The nature of the objective function can have a significant effect on the results of optimization [191]. Once the objective function has been calculated at each point in the initial simplex, the code then applies the Nelder & Mead search algorithm as described in Section 3.2.

# 3.4 Review of Scramjet Optimization Studies

Over the last decade or so, there has been a number of studies that have applied optimization techniques to the design of complete scramjet powered vehicles and components of scramjet engines. Common to most of these studies has been an efficient flow solver coupled to a gradient-search optimization algorithm. Some of the earliest work in this field was performed by the group of Baysal, Eleshaky & Burgreen [22, 23, 34] who used an efficient sensitivity-based optimization scheme with a quasi-analytical method of computing the sensitivity coefficients as described earlier in Section 3.1. They applied the optimization method to the design of a simplified two-dimensional scramjet-afterbody configuration for optimized axial thrust. Most of their work has been devoted to improving the optimization method, rather than applying the method to new design problems.

McQuade et al. [148] used a similar efficient optimization technique to that of Baysal et al. for the design of a complete two-dimensional scramjet flight vehicle which was also optimized for thrust. However, they used a more general finite-difference approach for calculating sensitivity derivatives. The efficiency of their scheme is a result of calculating objective functions from approximate flow solutions rather than computationally intensive CFD solutions. The optimization scheme starts by computing a flow solution for an initial design using an implicit Euler flow solver. This flow solution is then used to construct approximate flow solutions of designs determined by the optimizer as is searches for the optimum design. The approximate flow solutions are calculated using approximate aerodynamic analysis techniques such as the method of characteristics, quasi-one-dimensional isentropic flow analysis, and oblique shock relations. As the design moves away from the initial design, the accuracy of the approximations deteriorates until a predefined limit is is reached. When this limit is reached, a new Euler flow solution is calculated and the optimization cycle begins again. The optimization scheme is very efficient, however, the use of approximate analysis techniques (known as global-local approximations (GLA)) limits the application of the optimization scheme to relatively simple flows.

Approximate analysis techniques were also used in the optimization study by O'Neill & Lewis [138] where they utilised the wave-rider concept to remove the need for iteratively computing CFD flow solutions. The geometries of wave-rider vehicles are determined by streamline tracing surfaces through flow-fields generated by some simple geometric object. In this study, a flow-field generated by a cone at a zero degree angle of attack in hypersonic flow was used to determine the surface profile of a three-dimensional wave-rider geometry which was integrated with a scramjet engine. The surface pressure

#### 3.4 Review of Scramjet Optimization Studies

of the wave-rider geometry that was unaffected by the scramjet engine, was simply extracted from the flow-field solution once the surface profile and scramjet position were determined by the optimizer. The surface pressure on the scramjet engine itself was determined from approximate analysis tools such as those used in the study by McQuade *et al.* [148]. Design variables were selected to specify the geometry of the wave-rider extracted from the conical flow-field solution and the geometry of the scramjet engine integrated into the vehicle. The simplex optimization algorithm of Nelder & Mead [159] was used to determine the value of these design variables for maximum vehicle thrust and lift to drag ratio. The design approach used in this study was shown to be effective for designing complete three-dimensional scramjet flight vehicles with high lift to drag ratios. However, viscous and high temperature gas effects were ignored in the modelling of the gas flow. These effects can have a significant influence on the overall performance of a scramjet engine and cannot be ignored for practical design studies.

The three-dimensional nature of scramjet flow was addressed by Korte *et al.* [127] who designed a three-dimensional planar-sidewall scramjet inlet duct for optimal totalpressure recovery and minimum flow-field pressure distortion. An explicit, upwind, spacemarching Euler CFD code was used to perform all of the flow-field calculations required by the optimization algorithm, and a Navier-Stokes code was used to analyse the optimal designs. The design problem was formulated with only two design variables which described the curvature of the inlet side walls. With just two variables, a simple gradient mapping technique could be used to perform the optimization. The inviscid flow analysis was shown to result in curved-wall three-dimensional inlets of enhanced performance with respect to standard planar-sidewall inlet designs. However, a viscous flow analysis revealed that the optimized designs exhibited top-wall boundary layer separation.

A trade-off between vehicle complexity and flow-field modelling accuracy was made in the optimization study of Sabean & Lewis [191], where the design of a supersonic combustion ram projectile shape was explored. The study used a chemically reacting Eulerian flow solver to model the axisymmetric flow through the complete projectile. To make the optimization problem practical, they used a simplified two-step reaction model to simulate the combustion kinetics within the projectile. Viscous effects were also omitted in an effort to reduce the time required for a flow solution. A finite-difference, sensitivity-based, gradient-search optimization algorithm was used to find optimum projectile geometries for maximum thrust, maximum speed over a finite flow length, and maximum acceleration. The study showed that the choice of the objective function had a significant effect on the benefits of optimization.

The applied scramjet optimization examples discussed in this section all used a gradientsearch optimization algorithm and the inviscid Euler equations to model the flow in the design process. Some studies also used simplified flow analysis techniques to increase the computational efficiency of the design process. Gradient-search methods were used in preference to stochastic optimization methods primarily because the studies were concerned with refining an initial aerodynamic geometry that was either well constrained, or known to be close to the optimum design. Simplified flow-analysis was used because of the complex nature of the flow within a scramjet engine. At present, the computational simulation of the complete flow through and around three-dimensional scramjets, where viscous and high temperature effects are accurately modelled, is too computationally intensive to incorporate in an iterative design procedure. Unfortunately, viscous, high temperature effects are the mechanisms which are of prime importance in functional scramjet design. Consequently, due to limitations in computational performance, many of the scramjet optimization studies to date have been exercises in applying new and improved optimization methods to an interesting design problem.

The scramjet optimization study in this thesis is similar to those reviewed in that a gradient-search optimization algorithm is used to optimize the flow path geometry of a complete scramjet engine for maximum axial thrust. However, it differs in that viscous and high temperature chemical effects are accounted for to some degree in the modelling of the flow. By modelling these effects, a more realistic approximation of engine performance was hoped to be achieved. Therefore, the results of the optimization algorithm would provide more insightful information with regard to important design issues for practical flight-style scramjet engines. In order to make the iterative design problem practical, the computational modelling was simplified by optimizing an axisymmetric scramjet geometry rather than a full three-dimensional geometry, and excluding the optimization of the external cowl surface. The scramjet design concept examined was an axisymmetric wrap-around concept with a conical forebody. The engine concept is proposed to be used for second stage of a flight vehicle capable of placing a satellite into orbit. The design problem was simplified further by dividing the engine into two separate components where the inlet and the combustor/thrust surface are designed independently. The details of this design process are the subject of Chapter 4.

## 3.5 Review of Nozzle Optimization Studies

To date, most of the design optimization studies for hypersonic nozzles that are designed to produce uniform, parallel test-flow, have used a non-linear, least-squares, sensitivity-based, gradient-search technique for finding optimal nozzle contours [97, 125, 118, 222]. Of these, most have coupled the optimization algorithm with a PNS flow solver to perform the hypersonic flow calculations. The popularity of least-squares optimization is largely due to the rapid convergence characteristics of the technique for well posed optimization problems, and the original application of the technique to nozzle design by Huddleston

[97]. However, rapid convergence is achieved at the cost of calculating design-variable sensitivity derivatives which are used to form a Jacobian matrix. The many flow calculations required to form and update the Jacobian matrix can limit the techniques practicality for optimization problems with many design variables.

The focus of the optimization problem in hypersonic nozzle design is typically the section of the nozzle contour where expansion waves generated by the initial part of the nozzle are cancelled and the flow is made parallel, otherwise know as the "turning contour". This section of the nozzle is illustrated as the wall contour of region 3 in Fig. 3.3. The shape of the initial expansion of an axisymmetric nozzle up to the wall inflection



Figure 3.3: The three regions of a contoured supersonic nozzle.

point (region 2 in Fig. 3.3) is somewhat arbitrary if the remaining part of the nozzle can correctly cancel the expansion waves. However, it is wise to select a shape that does not generate strong waves so that the flow can be corrected easily with the turning contour. The analytical representation of the turning contour is an important part of nozzle contour optimization since the method used dictates how the optimization design variables are defined, the quality of the exit flow achievable in the final optimized design, and the scope of possible design solutions. Ideally, the representation of the turning capable of representing a large range of shapes.

One approach for representing the turning contour is to use a composite of a fixed set of basis functions which represent a finite number of possible design solutions within the design space [118]. The optimization algorithm then seeks the optimum composite of these basis functions to minimise the objective function. Convergence rates are high for this approach, however, the design space is limited by the shapes of the basis functions.

Another approach that explores a greater range of wall contours is to use a set of cubic splines that are joined continuously to define the nozzle contour [124, 120]. The unconstrained coefficients of the cubic splines represent the slopes at discrete points along the contour and are used as design variables. A correlation of the design variables with wall

slopes has been shown to improve the rate of convergence for analytical nozzle wall representations [125]. Also, the quality of the nozzle exit flow can be increased by increasing the number of cubic splines defining the wall contour since greater control is achieved over wave cancellation.

An alternative to using a set of cubic splines to define the nozzle turning contour is to use a single Bézier curve. Bézier curves are an attractive choice for representing wall contours in optimization problems because they can accurately represent complex shapes with relatively few control points (or knots). Bézier curves have the useful property of passing through the first and last control points, and the endpoint slopes are specified by the slope between the first and last pair of control points. These qualities make it simple to join them continuously to the initial contour of the nozzle. Slope-based design variables can also be applied to Bézier curves by using the slope between adjacent control points as design variables since, for slowly varying curves, the control points approximately map the path of the curve. Another characteristic of Bézier curves that make them attractive is the mathematical simplicity and efficiency of the curve formulation (see Eq. 2.103). Other, simpler methods for representing wall contours have been used in the literature [222], however, they generally do not provide sufficient control over the shape of the turning contour to produce high quality flows [34].

Once the nozzle contour has been analytically defined, a computational grid can be constructed to fit the contour, and a flow-field solution can be calculated with a CFD flow solver. Efficient space-marching PNS flow solvers are typically used to calculate the flow through hypersonic nozzles where many iterative flow calculations have to be performed [125, 118, 222]. Some nozzle optimization studies have also used time accurate Navier-Stokes solvers to model the subsonic contraction and throat where boundary layers may develop and have an influence on nozzle performance [118, 222]. The downstream (exit plane) solution of the NS solver is then used as an inflow condition for subsequent PNS flow calculations which are used to optimize the nozzle contour.

After a nozzle flow solution has been calculated, an objective function is evaluated using selected data from the flow solution. Objective functions are defined firstly so that they reflect the desired goals of the design and secondly, so that they exhibit a strong minimum (steep slope close to global minimum) when the design goals have been achieved. Typical design goals in nozzle optimization are to minimize the deviation in Mach number and flow angularity across the test core of the nozzle. The definition of an effective objective function that exhibits a strong minimum when these design goal has been achieved is not obvious. One possible definition of an objective function is the summation of the deviation in Mach number for all of the computational cells in the core flow at the exit plane (where the core flow is the nominally uniform flow issuing from the nozzle). Most studies have used this definition with variations for defining the boundaries of the core flow. Two approaches that have been used for defining the boundaries of the core flow have been to (i) use a fixed percentage of radial cells, which requires a prior knowledge of the core flow boundary [120, 118], and (ii) use a weighting function that exponentially decreases as cell Mach numbers deviate further from the design Mach number so that all the radial cells in the exit plane can be used [222].

It is common to also see in the literature a second objective function that quantifies the deviation of the centre line Mach number. The purpose of this function is to ensure that the axial derivative of the Mach number within the core flow is driven to zero such that the flow will not continue to expand or compress as it passes into the test flow region. Various approaches for the definition of the centre line Mach number objective function include; a summation of the design Mach number deviation of all the cells for a centre line segment upstream of the exit plane equal to  $\sqrt{M_{design}^2 - 1}$  times the radius of the exit core flow [118]; a summation of the Mach number deviation for all the axial cells where an exponential weighting function is applied to damp out the contribution of cells that deviate substantially from the design Mach number upstream of the core flow [222]; and summing the deviation of all the axial cell Mach numbers from a prescribed axial distribution [120].

Despite the popularity of using a centre line Mach number distribution in the definition of the objective function, it can be argued that the inclusion of a centre line Mach number objective function is not essential for effective nozzle optimization. In the limit of the core flow being parallel and at the design Mach number, the distribution of Mach number along the nozzle centre line from the point where the flow is first expanded to the design Mach number to the end of the nozzle, has to be at the design Mach number. Therefore, the inclusion of a centre line Mach number distribution function is not essential to the optimization problem if a flow angle function is included in the exit plane objective function. However, a centre line Mach number objective function may increase the rate of convergence.

Many of the ideas discussed in this section are used in the later half of this thesis to design a Mach 7 axisymmetric nozzle and a Mach 7 square cross-section nozzle for a small pulse flow wind tunnel. The design tool used to design these nozzles is similar to that used in the design studies mentioned at the start of the section where a PNS flow solver is coupled to a gradient-search optimization algorithm. However, the design tool used in this thesis differs in that the Nelder & Mead simplex optimization algorithm is used to perform the optimization rather than a more complex least-squares algorithm. The formulation of the design problem is also simplified somewhat by (i) using Bézier curves to define the nozzle wall surfaces, (ii) defining the core flow edge with an adaptive definition, and (iii) excluding an axial Mach number function in the objective function. The application of the design tool using this problem formulation for nozzle design are the topics of Chapter 5 and 7 where the axisymmetric and square cross-section nozzles are designed.

# **Design of a Scramjet Engine Flow Path**

In this chapter, the computational design tool discussed in Chapters 2 & 3, is applied to the design of an axisymmetric scramjet vehicle flow path. The scramjet vehicle considered could be used to form the second stage for a satellite launch vehicle similar to that shown in Fig. 1.1. The goal of the design task was to design a scramjet engine flow path that produced the maximum thrust for a given fuel injection rate, mass capture area, and flight condition. The design problem was formulated in a similar way to the scramjet optimization studies reviewed in Section 3.4, where the design variables define the geometry of the vehicle and the objective function quantifies the vehicle performance through a function of the total axial force. However, the scramjet optimization design problems presented in the current study differ from those reviewed in that the flow solver used to perform the flow-field simulations, sm3d, models turbulent boundary layer development along the internal walls of the flow path and the multidimensional finite-rate combustion process within the engine. The added modelling complexity of the flow solver was used to give a more realistic approximation of the flow behaviour and enhance the accuracy of the engine performance estimates.

The design task was simplified by designing the integrated forebody/inlet first, then designing the combustor/thrust surface (see Fig. 4.1). This approach is not ideal since the



Figure 4.1: Cross-section of the scramjet flow path to be optimized.

compressed flow produced by the inlet is coupled to the performance of the combustor and thrust surface. However, treating the inlet and combustor/thrust surface separately reduced the computational effort required and made the design of a complete vehicle flow path using the computational design tool practical.

The structure of this chapter is organised into seven sections that detail the theory, methodology and results of the axisymmetric scramjet design process. Sections 4.1 & 4.2 are a prelude to the design of the engine since they discuss the flight conditions for which the scramjet is designed to operate, the design constraints, and the computational modelling assumptions made throughout the design process.

The design of the inlet is covered in Section 4.3, where three inlets based on various concepts are designed. The computational design tool discussed in Chapters 2 & 3 is used to optimize one of these inlets for minimum drag. The other two inlets are comparatively simpler, and are designed using only the flow solver. Each inlet design is then assessed by comparing the total calculated drag, wall heat transfer, and stream thrust efficiency for the given design condition.

The design of the scramjet combustor and thrust surface is described in Section 4.4. The design issues associated with a scramjet combustor and thrust surface are initially discussed followed by a detailed description of the computational design of the combustor/thrust surface. The design was undertaken by first performing a parametric study of the combustor length. The results of this study were then used to design an initial combustor/thrust surface suitable for optimization. This initial design was then optimized for maximum axial thrust force using the computational design tool.

The chapter concludes with Sections 4.5, 4.6 & 4.7, which detail the results of a grid refinement study, an analysis of the complete optimized axisymmetric scramjet design, and a summary of the main findings made throughout the design study. Also presented in Section 4.7, is a list of recommendations for future scramjet engine research that are based on the results and discussion of the design study contained within this chapter.

#### 4.1 Design Conditions and Assumptions

The design condition for the scramjet stage was selected to be at a flight Mach number of 12 and at an altitude of 31.5 km (i.e. within the stratosphere). This condition was obtained from a proposed flight trajectory suggested by Billig [27] (see Fig. 1.3). A Mach 12 flight number was selected as the design Mach number because it is approximately the highest Mach number in the flight trajectory where the maximum temperature within the inlet boundary layer does not exceed the dissociation temperature for oxygen ( $\approx 2500$  K at 1 atm.) [27]. Therefore, the inlet flow can be reasonably modelled (in terms of drag estimates and shock positions) with the assumption that the flow is chemically frozen, thereby reducing the computational time required for an inlet flow solution. The justification for selecting a high design Mach number also comes from an observation made by Stalker [208] in his analytical analysis of the inviscid thrust obtained from a simple twodimensional Busemann biplane scramjet concept: "It has been found that the net thrust of a duct which is configured for maximum thrust at a particular design Mach number is reduced as it departs from this Mach number, but the reduction is much more serious for Mach numbers in excess of the design value than for those below it. This suggests that if a propulsive duct is to operate over a range of Mach numbers, then it is best to choose a design Mach number at the maximum end of the range." (p. 263).

All of the flow computations were performed using the axisymmetric formulation of the parabolized Navier-Stokes equations (see Appendix A) and the Baldwin & Lomax algebraic eddy viscosity turbulence model (see Section 2.9). A turbulent boundary layer was assumed to develop from the nose of the inlet and leading edge of the cowl since the unit Reynolds number of the free-stream at the design condition ( $\text{Re}_{\infty}/\text{m} = 4 \times 10^6$ ) is quite high. Also, it is likely that an actual flight vehicle will have boundary layer trip devices near the leading edge to ensure that the boundary layer becomes turbulent. A turbulent boundary layer can withstand a higher pressure gradient than a laminar boundary layer before separation occurs [142]. The walls of the vehicle were assumed to be convectively cooled to a constant temperature of 1000 K by pumping cryogenic hydrogen fuel from the storage tanks through channels under the aerodynamic surfaces prior to the fuel being injected into the flow.

The geometry of the scramjet engine modelled in this chapter was simplified by not including an isolator section between the inlet and the combustor. It is likely that scramjets, which are to operate over a wide range of flight speeds from low supersonic Mach numbers to high hypersonic Mach numbers (Mach 6 to 25), will require a constant area duct prior to fuel injection at the beginning of the combustor. This duct is known as an isolator [48, 27]. The function of the isolator is twofold. Firstly, it gives the scramjet engine the capability of operating as a ramjet at low flight Mach numbers where the addition of heat into the flow through combustion can cause the combustor core flow to become subsonic (known as thermal choking). When choking occurs, a normal shock wave develops that travels upstream and forms a stationary normal shock train in the isolator. As long as the pressure rise due to combustion is not too great, the shock train will remain in the isolator and the engine will function as a ramjet with subsonic combustion [27]. However, "unstart" will occur if the pressure rise is too great causing the normal shock train to travel up through the inlet.

The second function of the isolator is to help prevent inlet "unstart" due to boundary layer separation caused by adverse pressure gradients in the combustor duct even when operating as a scramjet. If the pressure increase due to combustion occurs too rapidly, the boundary layer will separate and cause the pressure rise to propagate upstream through the boundary layer. Without an isolator, the pressure increase may result in the formation of a normal shock that travels upstream through the inlet and causes the engine to unstart. With an isolator upstream of the combustion chamber, the pressure increase in the boundary layer can be achieved with an oblique shock train which leaves the core flow supersonic.

Although an isolator will probably be required in a practical scramjet engine, a scramjet design incorporating an isolator is not considered in this chapter because the scope of the study does not include the issues of low Mach number operation and thermal choking.

As stated earlier, the assumption is made that oxygen does not dissociate appreciably within the inlet boundary layers for a flight condition of Mach 12. However, it is reasonable to expect that a small amount of dissociation may occur close to the downstream end of the inlet where the boundary layer temperatures are the greatest. Small amounts of atomic oxygen can significantly reduce the ignition delay time [83] within the combustor, particularly if the boundary layer flow is mixed with the fuel. However, at high flight Mach numbers (M>10), where the compressed gas entering the combustor is well above the auto-ignition temperature of hydrogen mixed with air, a more important issue than ignition delay may be the mixing of the fuel with the air [83].

Indeed, it is possible that the rate of combustion within a high Mach number combustor is entirely mixing controlled [183]. Little experimental work has been conducted in the field of high Mach number mixing due to a lack of test facilities capable of simulating the flight speeds at the upper end of a scramjet's flight corridor [27]. Consequently, computational methods are often used for the design and analysis of potential injector strategies. However, injection and mixing of fuel in a supersonic air-stream is a very complex problem that is difficult to simulate accurately [239, 73, 178, 128]. The flow associated with hypersonic injection and mixing is generally three-dimensional and requires a large amount of computational resources to resolve the flow patterns inherent with mixing.

Modelling fuel injection and mixing in the current study would increase the time required for a flow simulation of the scramjet to a degree where design optimization, requiring many flow simulations, would become impractical. Therefore, the assumption/simplification was made in the flow simulations for the combustor/thrust surface, that fuel is injected at the start of the combustor and is instantaneously mixed with the air-stream. This was done in the flow solver by simply adding the appropriate mass, momentum, and energy source terms in the governing equations (see Eq. 2.5). Fuel is only added to a central region, half the width of the combustor to simulate the ideal mixing of fuel from a central strut injector (see Section 4.4.2). Since fuel is not added directly into the boundary layer flow, assuming the inlet flow to be chemically frozen was thought to have little or no effect on the heat release of the combustion process.

Molecular diffusion was not modelled in the flow simulations for the combustor/thrust surface because the effects of molecular diffusion were assumed to be negligible and detrimental to the performance estimate of the engine. Diffusion was thought to be negligible because the velocity of the combustor flow for the Mach 12 flight condition is very high ( $\sim 3300 \text{ m/s}$ ) so the residence time is very short. Also, the combustor mixing efficiency is over estimated by assuming ideal fuel injection, therefore, modelling diffusion would only increase the error associated with the mixing efficiency. It has also been claimed that in the case of scramjet flow, the diffusion terms have little effect on overall afterbody forces compared to the convective terms [58].

### 4.2 Thermochemical Modelling

At an altitude of 31.5 km, the mean pressure and temperature of the atmospheric air is approximately 957.4 Pa and 228 K respectively [158]. The composition of the air at this altitude was assumed to be the same as the mean composition of clean, dry air at sea level which is listed in Table 4.1 (assuming the mass of the unlisted species that are present in the atmosphere are made up with the mass of the Argon). The composition of the

Table 4.1: Mean composition of dry air at sea level by mass [158].

Species	mass fraction
$N_2$	0.7552
$O_2$	0.2314
Ar	0.0134

major constituents of air is known to vary little below an altitude of 90 km [158], so using this composition for the gas entering the scramjet is a reasonable assumption. However, the concentration of species such as  $O_3$ ,  $H_2O$ , O and  $NO_2$  varies considerably within the stratosphere (<50 km) depending on altitude, climate, time of day and pollution levels. These molecules are present in only minute quantities at 31.5 km and there is not enough to significantly alter the sound speed of the air by including them in the mixture given in Table 4.1. However, air vitiated with small amounts of these molecules can have a significant effect on ignition delay times in scramjet combustors particularly at low flight Mach numbers [102, 163, 83]. Since the focus of this study was not to model ignition delay to a high accuracy, the thermodynamic model of the air flow was limited to the species shown in Table 4.1.

A state of thermodynamic equilibrium was assumed throughout the entire scramjet flow-field for the calculations presented within this chapter. The equilibrium gas state was modelled using curve fits from the NASP Reaction model report [163]. The curve fits are functions of static temperature for specific heats that are valid up to temperatures of 6000 K which is well above the maximum temperature expected within the combustor of the scramjet (see Appendix B for curve fit data).

Thermodynamic equilibrium in a gas mixture is a state where the maximum relaxation time is small, in comparison to the characteristic fluid time scale. The maximum relaxation time for a gas mixture is the maximum time for each excited energy mode of the atoms and molecules making up the gas mixture, to come to a steady state after a change in the internal energy of the gas mixture. For the gas mixture flowing through the scramjet engine, the slowest mode of energy to relax after a change in the internal energy is the vibration mode since the temperature of the gas is never high enough to excite the slower electronic modes. Translational and rotational relaxation times of all the atoms and molecules present within the flow are generally very short and can be safely considered to be in equilibrium for all conditions within the scramjet. Also, thermodynamic equilibrium can be assumed for all the energy modes up to a temperature of approximately 1500 K where the vibrational energy contribution and relaxation time of the oxygen molecules can become significant [81]. Since the maximum core flow temperature within the inlet of the scramjet was not designed to exceed 1300 K, and the hotter boundary layer flow has a large time scale because of the reduced flow velocity, the assumption of thermodynamic equilibrium for the inlet flow calculations is reasonably valid.

However, the core flow within the combustor of the scramjet engine was expected to reach a static temperature of approximately 2100 K. At this temperature, most of the oxygen molecules have reacted with the fuel or have dissociated into atoms, and the vibrational modes of nitrogen become the most dominant contributers to vibrational energy. To determine the vibrational relaxation time,  $\tau_{vib}$ , for molecular nitrogen at this temperature, an empirical expression derived by Millikan and White [154] can be used:

$$p \tau_{\rm vib} = \exp[a(T^{-1/3} - b) - 18.42]$$
 atm.sec (4.1)

In this relation p is the static pressure in atmospheres and the parameters a and b can be expressed for many gases by the simple expressions

$$a = 0.00116 \ \mu^{0.5} \ \theta^{1.333}, \quad b = 0.015 \ \mu^{0.25}$$
 (4.2)

The variable  $\mu$  is the equivalent molecular weight between two colliding particles in g/mol, and  $\theta$  is the characteristic vibrational temperature of the oscillator molecule in degrees Kelvin. For an air and hydrogen gas mixture, the collision resulting in the slowest vibrational relaxation time is a molecular nitrogen-nitrogen collision. The equivalent molecular weight for this collision is 14 g/mol and the characteristic vibrational temperature is 3395 K (data obtained from [154]). For a temperature of 2100 K and at an estimated maximum combustor pressure of 2.3 atmospheres (obtained from preliminary

#### 4.2 Thermochemical Modelling

calculations), the vibrational relaxation time given by Eq. 4.1 is approximately 224  $\mu$ s. The velocity of the combustor flow is approximately 3200 m/s which means that the flow must travel 0.7 metres before the vibrational mode of nitrogen comes to an equilibrium state. However, this length was expected to be of the same order as the combustor length. Therefore, the combustor flow would be in a state of vibrational non-equilibrium which is not what was assumed within this chapter.

There are several reasons why thermodynamic (and hence vibrational) equilibrium was assumed within the combustor despite the indication that the flow would not be in equilibrium. Firstly, modelling thermodynamic non-equilibrium flow in a flow solver requires the implementation of a multi-temperature thermodynamics model which can be quite complicated and computationally intensive [169, 133, 146, 35]. Due to time constraints and the extra computational time required to complete the optimization flow calculations for the combustor/thrust surface, such a model was not added to the *sm3d* flow solver during the course of this thesis. Secondly, the fraction of the internal energy that is composed of vibrational energy for nitrogen at a temperature of 2100 K is only 14% (see equations in reference [9]). Therefore, the approximate maximum error in mixture internal energy is only  $0.14 f_{N_2}$ . Lastly, the amount of energy released through combustion was large in comparison to any internal energy errors associated with vibrational relaxation. For nitrogen flowing through the combustor at a temperature of 2100 K, the flow rate of vibrational energy is approximately 6 MJ/s. The rate of stoichiometric heat release within the combustor is approximately 80 MJ/s.

Of all the thermochemical processes possible in a gas, chemical reactions (including ionization) take the longest time to equilibrate. Since the vibrational energy modes of nitrogen are in non-equilibrium within the combustor, it can be inferred that the combustion process is also in a state of non-equilibrium. Therefore, to model the combustion process with reasonable accuracy, a finite-rate reaction model was included in the flow solver. Including a reaction model enabled the investigation of the hypothesis that there would be a trade-off between rapid expansion of the combustion products to avoid viscous losses and the slow expansion needed to allow optimum combustion.

The complexity of the finite-rate reaction model has a strong bearing on the amount of computational time required for a flow solver to produce a flow solution. Therefore, for optimization studies where flow solution time is a major concern, efficient reaction models are needed. Reaction models for hydrogen combustion in air can be significantly simplified by omitting reactions involving atomic nitrogen and nitrogen molecules. Reactions involving nitrogen have a strong effect on heat release in the combustion and expansion process when temperatures in the combustor reach the dissociation temperature of nitrogen ( $\approx 4000$  K). Also, reactions involving nitrogen (particularly NO) significantly effect the ignition delay for flight Mach number greater than 12 [102]. However, since the ac-

curate modelling of ignition delay was not a prime focus of this study and the maximum temperature in the combustor is not expected to be above 3000 K, excluding reactions involving nitrogen was thought to be a valid simplification. Various hydrogen/oxygen finite-rate reaction models were assessed in Appendix C with the aim of identifying an accurate and computationally efficient model to be used in the design calculations. Of all the models assessed, the 8 reaction, 7 species reaction model of Evans & Schexnay-der [61] was identified as being the most computationally efficient model. However, the accuracy of the model was poorer than the other models assessed. The model was subsequently modified to increase its accuracy to the same level as the other models for the flow condition studied, and then implemented in the flow solver to perform the combustor/thrust surface flow calculations.

#### 4.3 Inlet Design

The design of the inlet for the axisymmetric scramjet stage was undertaken by designing three different inlets and selecting the design with the best performance. The selection criteria was based on the drag generated by the inlet and its susceptibility to boundary layer separation. One of the inlets was designed with a bent cowl to reduce the strength of the injected shocks and hence reduce the likelihood of boundary layer separation. The computational design tool discussed at the beginning of this thesis was used to optimize the design of this inlet for minimum axial drag.

The design process described above is presented in the following three sub-sections. The first sub-section discusses some inlet design issues and introduces the axisymmetric inlet design concepts that are considered in this study. The next sub-section details the design of three inlets that are based on the design concepts of the previous sub-section. The final sub-section presents a quantitative performance assessment of all three inlets to determine the most practical design. The assessment consists of total calculated drag, wall heat transfer, and stream thrust efficiency comparisons for each design.

#### **4.3.1** Inlet Design Concepts

The design of a scramjet inlet<sup>1</sup> is conceptually simple. Its purpose is to compress the oncoming gas to a pressure and temperature that are suitable for auto-ignition and sub-sequent combustion with hydrogen fuel, and direct it into the combustor using inclined body surfaces that generate oblique shocks. However, the design of an efficient inlet that can be practically implemented on a flight vehicle is not simple. At high Mach numbers,

<sup>&</sup>lt;sup>1</sup>For the remainder of this chapter, the inlet refers to the integrated forebody and scramjet inlet.
problems arise due to boundary layer separation, high surface skin friction & heat transfer, and high dynamic loads on the vehicle.

A good inlet design is usually characterized in the literature as having low drag and a high compression efficiency [84]. Compression efficiency is typically a measure of the total pressure that is conserved through a compression processes or flow work lost due to entropy gains (which implies a decrease in total pressure). An inlet that has a high compression efficiency, produces compressed flow that can do more expansion work and hence produce higher vehicle thrusts as it is expanded over a thrust surface. In the case of a scramjet inlet, the major sources of total pressure loss are shocks and boundary layer skin friction & heat transfer.

Losses due to shocks can be minimised by reducing the strength of the shock and/or correspondingly increasing the obliqueness of the shock. Ideally, an axisymmetric scramjet inlet would be designed with a shock free, or smooth isentropic compression surface with a long sharp nose (see Fig. 4.2 (a)). However, such a design is impractical because of the low structural strength and excessive viscous drag and heat transfer along the centre body. Therefore, practical axisymmetric hypersonic inlet concepts have noses or forebod-



Figure 4.2: Several inlet design concepts for an axisymmetric scramjet.

ies with half angles that are large enough to withstand high dynamic loads [143]. These forebodies generate oblique shocks which compress and turn the flow into the scramjet combustor.

The simplest application of this idea is an inlet composed of a single cone with a cowl aligned with the free-stream (see Fig. 4.2 (b)). The shock emanating from the tip of the cone compresses the oncoming flow and directs it up along the surface of the inlet. Ideally, the cone shock reflects off the tip of the cowl and redirects the flow uniformly into the

combustor. At on-design conditions, the reflected shock is cancelled at the elbow of the inlet (labelled ' $\alpha$ ' in Fig. 4.2) so that the combustor flow is shock free and uniform. Shock free and uniform flow entering the combustor has been suggested as being beneficial for optimum combustor performance [138]. A possible problem with this inlet configuration at high Mach numbers is boundary layer separation. At high Mach numbers, the pressure ratio across the reflected shock can be high enough to cause boundary layer separation [141, 144] which can lead to choking and engine unstart.

One possible way of avoiding the problem of boundary layer separation is to decrease the cone angle (see Fig. 4.2 (c)). Decreasing the cone angle weakens the strength of the oblique shocks and therefore reduces the likelihood of boundary layer separation. Compressing the inlet flow with many weaker shocks rather than fewer stronger shock is advantages because less total pressure is lost for a given compression ratio. However, this benefit can be nullified in long inlets due to the excessive drag and heat transfer.

The short cone inlet can be modified for high Mach number flows where boundary separation can be a problem by bending the cowl lip down as shown in Fig. 4.2 (d). Bending the cowl lip towards the compression surface, reduces the strength of the initial reflected shock and distributes the compression processes more evenly across the down-stream shocks. Interestingly, this axisymmetric inlet concept has been used for the ram inlet of the Pratt & Whitney J58-I after-burning turboramjet engine used in the Lockheed SR-71 and the inlet for the recently flown CIAM-NASA Mach 6.5 Scramjet [184]. The disadvantage of this approach is the increased form drag for a given mass capture area due to the bent cowl but, because a stronger initial shock can be generated at the nose cone without causing boundary layer separation, the length of the inlet can be substantially reduced thereby reducing drag and total pressure losses caused by skin friction and heat transfer.

From this discussion, it is not clear which design concept could be practically implemented as a design for the Mach 12 scramjet. The only concept that can be ruled out immediately is the isentropic inlet because of the impractical length and sharpness of the inlet forebody. In the following sub-section, three inlets are designed for the Mach 12 scramjet using the remaining concepts to determine the more practical design concept. The flow generated by each of the designs is assessed and a quantitative analysis of drag and heat transfer is undertaken to determine the more efficient design at the Mach 12 condition. It should be noted that inlet concepts with boundary layer bleeds were not explored in this study due to the added complexity of modelling the multiple flow paths. Outside of the issues addressed here, boundary layer bleeding is an effective way of minimising boundary layer separation problems and may need to be employed in practical inlet designs.

### 4.3.2 Multi-Shock Inlet Design

At the Mach 12 flight condition, Billig suggests [27] that the air entering the combustor (or isolator if the scramjet is to be operated at low supersonic speeds) should be at a temperature of 1300 K and be compressed to a pressure of at least 120 kPa. In the following investigation of the three multi-shock inlet concepts, it was not possible to match these conditions for all three inlets due to the varying lengths of each inlet. Therefore, each inlet was designed to match only the temperature of the core flow at the exit plane of the inlet with the temperature suggested by Billig. The temperature was selected over the pressure because of the greater sensitivity the temperature has to the ignition delay time at the Mach 12 design condition. The sensitivity was determined by differentiating an empirical correlation for the ignition delay time,  $\tau_i$ , derived by Huber *et. al* [96]

$$\tau_i = \frac{8.0 \times 10^{-9} \mathrm{e}^{\frac{9600}{T}}}{p} \tag{4.3}$$

where the pressure, p, is in atmospheres and the temperature, T, is in Kelvins. This relation has been shown to give good estimates of the ignition delay time determined by complex reaction models of hydrogen combustion in air [56]. Differentiating this equation revealed that the ignition delay time decreases at a rate of 0.109  $\mu$ sec per percent increase in pressure and 0.803  $\mu$ sec per percent increase in temperature at the design condition where the ignition delay is predicted as being 10.88  $\mu$ sec.

The first inlet designed was an inlet with a short single conical compression (the inlet concept shown in Fig. 4.2b). The design was determined by starting with a 20 degree (half angle) conical inlet with an internal cowl radius of 0.45 metres and combustor entry height of 11 millimetres (from the compression ratio suggested by Billig [27]). The inlet design also had a 0.1 metre constant area section leading into the combustor. A viscous flow solution was then calculated for this initial design using *sm3d*. The inflow conditions for the flow solution were,

$$\begin{split} \rho &= 0.01463 \; \mathrm{kg/m^3}, \quad u_x = 3634.0 \; \mathrm{m/s}, \quad u_y = u_z = 0.0 \; \mathrm{m/s}, \\ e &= 1.592 \times 10^5 \; \mathrm{J/kg}, \quad p = 957.5 \; \mathrm{Pa}, \quad T = 228 \; \mathrm{K} \end{split}$$

where the composition of the gas is given in Table 4.1. As stated earlier, the flow was assumed to be chemically frozen and in vibrational equilibrium. A computational grid containing 50 cells in the cross-stream direction and 5000 cells in the streamwise direction was used to discretize the computational domain (see Fig. 4.3). The grid was clustered towards the walls using a exponential clustering parameter of 1.01 (see Eq. 2.104) to give  $y^+$  values of 5.1 and 5.3 for the cells nearest the top and bottom walls at the exit plane



**Figure 4.3:** Computational mesh used for the cone type inlet. Note that only one in every 20 axial cells are shown.

respectively where

$$y^{+} = \frac{y\rho_{\text{wall}}\sqrt{\tau_{\text{wall}}/\rho_{\text{wall}}}}{\mu_{\text{wall}}} .$$
(4.4)

The  $y^+$  value is the distance away from the wall non-dimensionalized by a viscous scale of the fluid close to the wall. The edge of the viscous sublayer within a turbulent boundary layer is typically characterized by a  $y^+$  value of approximately 5 [129]. The convergence criteria for the flow solution was set to a density residual of 0.01%. A free-stream boundary condition was set along the top wall of the computational domain and switched to the constant temperature no-slip boundary condition where the initial cone shock first contacts the wall.

The cone angle and combustor entry height of the initial design were iteratively modified until the flow solution gave a core flow temperature at the exit plane of 1300 K and the shock that reflected off the cowl was cancelled at the inlet elbow. The iterative process was simple and did not require the use of an optimizer. The Mach contours of the resulting design are shown in Fig. 4.4. The cone half angle of the short inlet design was



**Figure 4.4:** An axisymmetric inlet design that uses the single cone inlet concept with contours of Mach number shown (20 contours from 0 to 12).

14.7° and the contraction ratio was 11.4. The average static pressure of the inlet outflow plane was calculated as being 74 kPa which is significantly lower than the target pressure

#### 4.3 Inlet Design

of 120 kPa. Also shown in Fig. 4.4 are the Mach contours of the external cowl flow. The flow-field over the external cowl surface was calculated with a separate flow simulation. The cowl thickness was fixed at 25 millimetres and the cowl tip had a wedge angle of  $10^{\circ}$ . A computational domain of 50 radial cells and 5000 axial cells was used to discretize the flow-field bounded by the external cowl surface, the axial plane where the inlet flow simulations were terminated and the external cowl shock. The cells were clustered towards the cowl surface using a exponential clustering parameter of 1.04 to give a y<sup>+</sup> value of the cell nearest the wall at the exit flow plane of 3.2. The same gas inflow properties and thermochemical assumptions used for the inlet flow simulation were used for the cowl simulation.

Even though the single cone inlet is quite short and the cone angle is large enough to maintain structural integrity (assuming a cone half angle of approximately  $15^{\circ}$  is a safe structural limit [143]), the rapid increase in pressure across the reflected inlet shock is likely to cause boundary layer separation. This assertion is based on a separation criterion proposed by Billig [27]. The criterion is based on the change in Mach number across a shock that impinges on a boundary layer and is given as

$$M_{\rm sep}^2 \leqslant 0.58M^2 \tag{4.5}$$

where  $M_{sep}$  is the Mach number that will cause separation downstream of a single oblique shock and M is the Mach number upstream of the shock. For the short conical inlet deign, the Mach number of the core flow prior to the reflected shock near the boundary layer on the cone surface is approximately 6.7, and the Mach number of the core flow after being processed by the reflected shock is 4.6 (see Fig. 4.4). Billig's criterion states that the minimum post shock Mach number allowable to maintain an attached boundary layer for Mach 6.7 flow is 5.1 . Therefore, it is likely that this inlet design will have boundary layer separation. The boundary layer did not separate in the flow calculations, however. This is because the governing equations used were the parabolized Navier-Stokes equations which do not permit upstream propagation of pressure waves within the boundary layer. The flow solver can not accurately predict boundary layer separation in the streamwise direction.

The next inlet concept that was assessed was the concept shown in Fig. 4.2(c) with a long multi-shock inlet. This multi-shock inlet design concept was applied to the Mach 12 design condition through a similar process to the one used for the short conical inlet. An inlet design with an internal cowl radius of 0.45 metres (see Fig. 4.5), a combustor entry height of 11 millimetres and a 0.1 metre constant area section leading into the combustor was also used as an initial design for finding a long inlet design that produced flow with the required exit plane temperature. The initial cone angle of the long inlet design was set

at 5°. The cone angle and combustor height were iteratively changed until the strength of every shock wave intercepting a boundary layer was not great enough to cause boundary layer separation (according to Eq. 4.5), and the core flow temperature at the entry to the combustor was 1300 K. The computational setup for this inlet design was the same as that used previously, however, 10000 cells were used to discretize the computational domain in the axial direction and the y<sup>+</sup> value of the cell nearest the cowl at the exit flow plane was 10.0. The cowl boundary condition was started at the point on the top edge of the computational domain where the initial forebody shock reflected.

The Mach contours for the long inlet design at the Mach 12 flight condition are shown in Fig. 4.5. The external cowl shock structure is also shown in this figure. The pre-



**Figure 4.5:** Mach number contour plot of a long conical inlet design that uses multiple shocks to compress the flow (NTS).

dominant features of the long inlet design are the excessive length and the thick boundary layers at the entrance to the combustor. Since weaker oblique shocks were used to compress the inlet flow for the long inlet design, the height of the combustor had to be significantly reduced to produce the high temperature core flow required for combustion. The combustor height for the long multi-shock design was only 8.4 millimetres compared to the short single shock inlet which has a combustor height of 20.1 millimetres. This significant reduction in combustor height was required to produce the high temperature core flow suitable for combustion. The larger compression ratio of this design results in a higher pressure at the combustor entrance ( $\sim$ 300kPa) which beneficially (but marginally) reduces the ignition delay time [96]. However, the increased compression surface length resulted in a substantial increase in drag due to skin friction. An assessment of the drag forces for all three inlet designs is given in the following sub-section. The cone half angle of this design was very small at 3.9° which is well below the desired 15° cone half angle for structural integrity.

Another problem with the long multi-shock inlet is the thickness of the boundary layers. As shown in Fig. 4.5, the boundary layers span the majority of the combustor height leaving only a small central region at the design temperature of 1300K. The boundary layer flow is considerably hotter and reaches a maximum temperature of 2448 K at the

#### 4.3 Inlet Design

exit plane. With so much of the flow at a higher temperature than the core flow, the engine is more susceptible to thermal choking when combustion occurs. Thermal choking occurs when the heat release due to combustion is great enough to cause a normal shock to form, thus resulting in engine unstart.

The last inlet design concept assessed was the inlet with a bent cowl shown in Fig 4.2(d). This concept is similar to the inlet design in the study performed by Ikawa [100]. The application of this concept to the Mach 12 design condition was more complicated than the previous two concepts and required the solution of an optimization problem using the design tool discussed in Chapter 3. The optimization problem was solved in two stages. First, an inlet design was optimized using a low resolution computational grid, then this design was used as the starting point for a high resolution optimization problem.

The design variables of the optimization problem defined the geometry of the inlet and the objective function was defined as the integrated surface drag due to static pressure and skin friction. The layout of the design variables is illustrated in Fig. 4.6 along with the constraining dimensions. As in the other two inlet designs, the capture area of the



Figure 4.6: Design variables for inlet optimization.

inlet was fixed by limiting the radial position of the cowl tip to 0.45 metres. However, to provide a bent cowl section, the radial position of the top wall of the combustor was fixed at 0.5 metres. This radial position was selected somewhat arbitrarily. Ideally, the radial position of the combustor would be set as a design variable in the optimization problem. The combustor entry duct height, h, would also need to be set as a design variable to maintain the desired combustor entry temperature. The optimization algorithm could then be made to find the correct combustor entry height by setting a penalty function for the core flow temperature. This approach was not taken in the present study because of the added problem complexity required.

To maintain the structural integrity of the inlet design, the initial cone angle was fixed at 15°. This was done by expressing the radial coordinate of point "a" (see Fig. 4.6) as

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a function of the axial design variable, dv[0]. Another constraint was placed on the inlet duct section bound by the internal bent cowl surface and the two corner points on the inlet body that are used to cancel shocks. This duct section was maintained at a constant area (through functions of the radial positions) to ensure no shocks or expansions would be produced when the first reflected shock is completely cancelled on the first corner.

The initial design variables for the optimization problem were determined from a flowfield calculation of a  $15^{\circ}$  half angle cone at a zero degree angle of attack with the design conditions used as the free-stream conditions. The calculated shock position gave the initial location of the cowl tip as shown in Fig. 4.7(a). The combustor height, *h*, was



**Figure 4.7:** Method for working out initial design variables for inlet optimization: (a) the initial  $15^{\circ}$  cone flow simulation; (b) the scheme for working out the initial design variables; (c) the low resolution grid for the initial optimization design.

initially set to give the same cross-sectional area at the combustor entry as the short conical inlet described previously. The remaining design variables were determined using the strategy shown in Fig. 4.7(b). The combustor entry height was then refined through an iterative process using low resolution viscous flow calculations to get the correct average combustor entry temperature. The final combustor entry height was calculated as being 14.9 millimetres.

#### 4.3 Inlet Design

The computational domain for the low resolution flow solutions was discretized with 20 cells in the radial direction and 5000 cells in the axial direction (see Fig. 4.7(c)). The cells were clustered radially towards the top and bottom of the domain using a fairly strong exponential clustering parameter of 1.04, and the cells were also clustered axially about the streamwise location x = 1.70 m with a relatively weak clustering parameter of 4.0 (see Eq. 2.107). As with the other inlet simulations, the edges of the domain that coincided with the inlet surfaces were set to a no-slip constant temperature boundary condition with a wall temperature of 1000 K. A CFL number of 0.45 was used to maintain numerical stability and the convergence criteria was set to a maximum density residual of 0.01%. The objective function was defined as the total integrated drag on the inlet (not including the external cowl surface) due to static pressure and skin friction, and the initial perturbations of the design variables were all set to 50 millimetres.

The optimization algorithm required approximately 12.7 CPU hours using one processor of the SGI Origin 2000 (see Appendix G) and 95 iterations to optimize the low resolution inlet to a converged design. The optimization convergence criteria used was a simplex objective function variance of 1.0 Newtons (or  $\approx 0.01\%$  of total drag) (see Section 3.2 for an explanation of the convergence criteria). The total drag for the converged design solution was calculated as being 10.5 kN compared to the initial design solution drag of 11.4 kN. The magnitudes of these drag estimates were expected not to be accurate because of the low grid resolution in the radial direction. However, the trends in the change of drag force with shape were assumed to be correct. The y<sup>+</sup> values of the cells nearest the top and bottom walls at the exit plane of the optimized inlet flow solution were calculated as being 21 and 22 respectively. These values are quite large and indicate that the viscous sublayer was poorly resolved. The low resolution optimization case was primarily used to reduce the computational time required for the high resolution optimization case.

The optimized low resolution design was used as the starting point for the high resolution optimization problem. The computational domain for the high resolution problem was discretized with 50 cells in the radial direction and 10000 cells in the axial direction. The clustering parameters and all of the other computational settings for high resolution computations were the same as those used previously for the short conical inlet computations. Since the initial design was expected to be quite close to the global minimum, the initial perturbations of the design variables were reduced to 10 millimetres.

The optimization algorithm took 30.4 CPU hours to compute the optimal high resolution inlet design. The convergence criteria was reached after 49 iterations were performed with an objective function variance of 1.0 Newtons. Table 4.2 shows the values of the initial and optimized design variables where the initial design variables are the variables used to start the low resolution optimization. The Mach contours for the optimized design flow

	dv[0]	dv[1]	dv[2]	dv[3]
Initial	0.906	1.455	1.611	1.711
Optimized	1.038	1.414	1.703	1.720

**Table 4.2:** The initial and optimized design variables for the inlet design with the bent cowl (variables in metres).

solution are shown in Fig 4.8 along with the Mach contours for the initial design which were obtained from a high resolution simulation of the initial design. Also shown in Fig.



**Figure 4.8:** Mach contours of the initial (upper half) and optimized (lower half) inlet designs. There are 30 contour levels of Mach number ranging from 0.1 to 11.9

4.8 are the external Mach contours produced by the bent cowl for the initial design and the optimal design. A separate flow solution was performed to calculate these Mach contours and the drag on the external surfaces of the bent cowl. The computational domain for these simulations started at the cowl tip and ended at the same axial position as the computational domain used for the inlet optimization. A grid with 50 cells in the radial direction and 2500 cells in the axial direction was used for these flow calculations. Each grid was clustered towards the cowl surface and towards the inflow plane. A constant temperature wall was set as a boundary condition along the cowl surface and the Baldwin & Lomax turbulence model was used to model the growth of a turbulent boundary layer from the cowl tip.

The optimization of the initial inlet design resulted in a 17.3% reduction in the total amount of drag which is a considerable improvement. The total axial drag force (including

the contributions due to the cowl) for the initial and optimized design were calculated as being 21.4kN and 17.7kN respectively. Most of this drag reduction was achieved through cancellation of shocks, minimisation of the inclined downstream compression surface exposed to the high pressure flow, and minimisation of the cowl angle. The position of the downstream shocks for the initial and the optimal designs is shown in the pressure contour plots of Fig. 4.9. An analysis of the Mach number jump across all of the shocks



**Figure 4.9:** Contours of pressure for the initial and optimized inlet designs. There are 30 contours of static pressure ranging from 1kPa to 130kPa.

in the optimal design flow solution showed that no shocks were strong enough to cause boundary layer separation (according to Eq. 4.5). The weakening of the shocks can be observed in Fig. 4.9 where the optimized design produces shocks that are generally more oblique in comparison to the initial design. The average static pressure of the flow at the exit plane of the optimized inlet is approximately 104 kPa which is close to the design goal of 120 kPa. Since the shocks were cancelled on entry to the combustor in the optimized design, the flow into the combustor is uniform. Uniform combustor entry flow has been claimed to be beneficial for effective combustion [138], however, this may not be the case at low flight Mach numbers where shock waves entering the combustor may be relied on to form high temperature regions, or "hot-spots", which can be used as a source of ignition [27].

The most practical inlet design out of the three designed in this section appears to be the inlet with the bent cowl. The short inlet was shown to generate a strong shock which may cause the downstream boundary layer to separate at the Mach 12 design condition. Also, the long inlet has a slender nose with a small cone half angle that was thought to be insufficient to maintain structural integrity. The optimized bent cowl inlet on the other hand, is not likely to suffer from boundary layer separation at the Mach 12 flight condition and the conical half angle is great enough to maintain structural integrity. Therefore, as previously done by CIAM-NASA for the Mach 6.5 scramjet [184], the optimized bent cowl inlet design was selected as the inlet for the scramjet module designed in this chapter. The flow solution at the exit plane of the optimized inlet design was used as the inflow condition for the scramjet combustor/thrust surface flow simulations in following sections of this chapter.

# 4.3.3 Performance Assessment of Inlet Designs

This section provides a quantitative analysis of the drag, heat transfer and efficiency associated with the three inlet designs described in the previous section. Estimates of total drag for each design were calculated by integrating the pressure and skin friction over all of the wetted inlet surface area including the external cowl surface. The total heat transfer was also calculated by integrating the heat transfer over the wetted area. Both of these quantities were calculated by the flow solver in the process of calculating the flow solution. The final quantitative measure used to assess the inlet performance was an efficiency term which is based on the fraction of the flow thrust power lost due to irreversibilities in the flow. This idea for efficiency was obtained from a recent study performed by Riggins *et al.* [177]. The efficiency term they derived is a truly second-law based efficiency term that takes into account all of the coupled and uncoupled losses present in the flow. As a result, it is a general and meaningful parameter that can be used to assess the performance of many types of thrust producing devices [175].

The efficiency is a ratio of the available or useful propulsive work of the flow at the exit plane of a flow device and the useful propulsive work of the flow entering the device. The useful propulsive work at any point in the flow is considered to be the thrust work of the fluid after an isentropic expansion to some reference condition. In the case of the inlet, the streamtube at any point is isentropically expanded to the area of the streamtube at the inlet plane or capture area cross-section. The stream thrust efficiency can be expressed as,

$$\eta = \frac{\int_{e} (\rho u^2 + p) dA}{\int_{i} (\rho u^2 + p) dA}$$

$$\tag{4.6}$$

where the denominator integral is the stream thrust at the entrance to the engine (or the component being analysed) and the numerator integral is the expanded stream thrust for the station of interest. The denominator is the ideal (reversible) stream thrust of the flow at the exit plane of an inlet with no losses present in the flow (isentropic inlet). Therefore the efficiency given by Eq. 4.6 is a quantitative performance measure of the fraction of thrust

power lost due to irreversibilities [177]. An inlet with a high thrust efficiency produces compressed flow that has more thrust power available for conversion into work through the expansion process.

The stream thrust of the flow exiting the inlet was calculated by summing the individual stream thrust of every cell at the exit flow plane. Each cell's stream thrust was determined by first isentropically turning the streamtube associated with that cell back into the direction of the free-stream flow. This involves a cross-stream area change in the streamtube if the cell velocity vector is not parallel to the free-stream velocity vector. The streamtube is then expanded isentropically back to the reference area where the reference area is a fraction of the total inflow mass capture area. The fraction is equal to the mass flow of the individual cell divided by the total mass flow across the inflow plane. The stream thrust efficiency is then calculated using Eq. 4.6.

The integrated drag forces for all of the inlet designs presented in this chapter are shown in Table 4.3. The inlet and external cowl drag forces due to the static pressure (inviscid) and skin friction (viscous) are listed separately for each design. The tabulated quantities are all based on the results of the high resolution simulations and are for complete axisymmetric designs. The total heat transfer from the flow to the inlet (including the cowl), stream thrust efficiency, and overall dimensions of all the inlet designs are shown in Table 4.4.

Inlet type	Inlet		Co	Cowl		Total	
	Inv	Visc	Inv	Visc	Inv	Visc	
Short	8.42	3.32	0.70	0.35	9.12	3.67	12.79
Long	8.40	10.43	0.71	0.80	9.11	11.23	20.34
Initial bent	10.95	5.02	4.69	0.73	15.65	5.75	21.40
Optimized bent	8.80	4.66	3.52	0.73	12.31	5.39	17.70

**Table 4.3:** Drag of inlet designs in kN. "Inv" represents the component of drag due to static pressure forces and "Visc" represents the component of drag due to skin friction.

Table 4.4: Heat transfer, efficiency, and geometry of inlet designs.

Inlet type	Heat transfer	Stream thrust	Length	Internal vol.
	(MW)	efficiency (%)	(m)	(m <sup>3</sup> )
Short	3.36	96.3	1.64	0.32
Long	12.59	93.3	6.50	1.33
Initial bent	6.01	95.6	1.81	0.44
Optimized bent	5.51	96.1	1.81	0.44

Several interesting points can be made regarding the quantitative results presented in both these tables:

• Firstly, the viscous drag component of the long inlet is greater than the inviscid component. This result indicates that minimising the inlet length at the Mach 12 design condition is an important design consideration. It also indicates that modelling boundary layer development and taking into account viscous drag is essential for quantitative scramjet performance assessment.

• The net unoptimized bent cowl inlet drag was greater than the long inlet drag even though the long inlet has a larger viscous drag component (approximately double). The greater amount of drag is a result of the increased form area associated with the bent cowl design. This result highlights the importance of making hypersonic flight vehicles as slender as possible.

• The excessive heat transfer and skin friction levels for the long inlet design has a detrimental effect on the stream thrust efficiency. The levels are so great, that the irreversible processes of heat transfer and skin friction contribute a larger gain in entropy than the reduction in entropy from compressing the flow with weaker shocks. As a result, the long inlet has the poorest stream thrust efficiency.

• The optimization of the bent cowl inlet achieved a substantial reduction in overall drag (17.3%). As discussed in the previous section, this reduction in drag was achieved through cancellation of shocks, minimisation of the inclined downstream compression surfaces and minimisation of the cowl angle. Stream thrust efficiency was also improved by optimization since losses were reduced because of shock cancellation. However, only a slight improvement in heat transfer was achieved through optimization.

• Even though the short inlet and bent cowl inlet are of similar length, the total viscous component of drag for the optimized bent cowl inlet is substantially greater. The larger viscous component of drag is due to the increased cowl length. The short inlet has a cowl with an axial length of 258 mm and the optimized bent cowl has an axial length of 498 mm which is almost double. Interestingly, the external viscous drag on the cowl is approximately double as well. The optimized bent cowl inlet also has a greater inviscid component of drag which as discussed earlier, is due to the greater form area associated with the bent cowl design.

• The inlet design with the highest stream thrust efficiency was the short inlet design. Even though this is not a practical design because of the potential problems with boundary layer separation, the design demonstrates that the reduction of heat transfer and skin friction can be just as important as reducing the number and strength of shocks when trying to design an efficient inlet (in terms of stream thrust efficiency). The last part of the performance assessment for the inlet designs was an analysis of the axial skin friction distribution for the optimized inlet design. The skin friction makes up approximately 30% of the total drag force for the optimized design (excluding cowl drag), which is a significant proportion. Figure 4.10 shows the distribution of calculated skin friction force along the length of the inlet where the plotted skin friction value is equal to the axial component of the wall skin friction force per unit length. The figure



**Figure 4.10:** Plot of axial skin friction force distribution along the surface of the optimized inlet. The profile of the optimized inlet design is shown at the top of the figure.

clearly shows that the skin friction force is greatest at the downstream end of the inlet where the inlet joins the combustor. This results illustrates the need to make the high temperature and pressure regions of the scramjet as short as possible in order to minimize skin friction. Another feature of the plot is the gradual increase in skin friction force moving downstream along the conical forebody. Most of the axial increase in skin friction is due to the increase in surface area as the cone radius increases rather than an increase in wall shear stress.

At the downstream end of the inlet, the flow is effectively contained within two concentric cylinders which give a high surface area to volume ratio. Consequently the skin friction is very high. A different scramjet inlet concept that would result in a lower skin friction force (assuming wall shear stress levels are the same) would be a funnel type inlet with a cylindrical combustor as shown in Fig. 4.11. The major reduction in skin friction would be within the combustor where the wall shear stress levels are the highest. For a



Figure 4.11: An internal axisymmetric scramjet concept.

given combustor cross-sectional area, the ratio of the surface area for a concentric cylinder type combustor to the surface area of a cylindrical type combustor is,

increase in surface area 
$$= \frac{(r_2^2 - r_1^2)^{\frac{1}{2}}}{(r_2 - r_1)}$$
 (4.7)

where the radiuses,  $r_1$  and  $r_2$ , are the inner and outer radii of the concentric cylinder type combustor. For the exit plane radii of the optimized inlet, the surface area ratio is approximately 8.1. Therefore, a substantial reduction in internal skin friction may be achieved if the scramjet is designed with a single cylindrical duct type combustor. A similar reduction would be achieved for the heat transfer.

# 4.4 Combustor/Thrust Surface Design

The design of the combustor and thrust surface for the axisymmetric scramjet stage was carried out by first undertaking a computational parametric analysis of the combustor length for an initial baseline design. The purpose of the parametric study was to approximately identify the optimal length of the combustor for premixed fuel injection. A parametric approach was used, rather than formulating an optimization, problem because it was believed that the gradient-search optimizer would not cover a large enough design space to investigate combustor designs that were very long and very short. It should be emphasised that the intention of the parametric study was only to identify an approximate optimal combustor length, since the actual optimal combustor length is coupled to the design of the thrust surface. The results of the parametric analysis were then used to specify an initial design that was subsequently optimized for maximum thrust using the optimization design tool presented at the beginning of this thesis. The optimization of the

#### 4.4 Combustor/Thrust Surface Design

combustor/thrust surface design was performed by solving only a single high resolution optimization problem since a low resolution computation of the flow would substantially under-estimate the skin friction. As discussed in Section 4.3.3, the skin friction within the combustor is expected to be high and would, therefore, have a strong influence on the results of the optimization.

The remainder of this section details the design procedure described above in three sub-sections. These sub-sections are prefaced by a sub-section that discusses some scramjet combustor/thrust surface design issues to provide an introduction to the following design study. The first of the three design sub-sections describes the assumptions and constraints used throughout the design process. Following this sub-section, the computational parametric analysis of the combustor length for an initial baseline design is described. Finally, the last sub-section presents the methodology and results for the optimization of the combustor/thrust surface. Within this sub-section, the performance of the initial and optimized designs is assessed and compared.

# 4.4.1 Discussion of Design Issues

The primary goal of the combustor and thrust surface of a scramjet is to extract energy from the combustion process and to use this energy to perform the maximum amount of work on the vehicle through expansion of the exhaust gases. The attainment of this goal is hampered by flow losses, inefficiencies and design constraints, which are often unavoidable in practical engine designs. Many of the dissipative losses associated with the inlet section of the scramjet, such as friction, flow separation and shock losses, are also prevalent in the combustor and nozzle. Additionally, the performance of the combustor and thrust surface is degraded by inefficiencies associated with fuel injection and mixing, finite-rate combustion kinetics, and incomplete combustion. Together, these loss mechanisms and the complex flow processes within the scramjet make up a highly coupled flow system that is not easily decomposed and analysed. In this section, some of the design issues associated with the combustor and thrust surface of a scramjet are detailed.

As stated in Section 4.1, the assumption is made that the hydrogen fuel is perfectly mixed with the air-stream at the injection point. The details of modelling injection and mixing have been deliberately avoided because hypersonic fuel injection and mixing in scramjet combustors is a very complex design issue [54, 48], particularly for high Mach number flows [176].

Although the mechanisms of hypersonic mixing are not modelled in the design of the combustor, the effects of finite-rate combustion are included. Inefficient finite-rate combustion (or incomplete combustion) of the fuel that is mixed with the air-stream is one of the major sources of thrust loss in a scramjet engine [177]. To initiate combustion,

the temperature and pressure of the air entering the combustor duct must be high enough to cause the hydrogen-air mixture to ignite and react in less time than the residence time of the flow in the combustor. Typically, temperatures and pressures of at least 1000 K and one atmosphere will cause combustion to occur and at a fast enough rate. For a given flight condition, the temperature and pressure of the flow entering the combustor are entirely dependent on the geometry of the inlet. The geometry of the combustor and expansion nozzle have a strong bearing on the completion of the combustion reaction and the amount of energy extracted out of the combustion process.

Once ignition has occurred, the temperature and pressure of the reacting gas rapidly increases as the exothermic reactions take place. As the reaction process continues, the concentration of intermediate radicals involved with combustion increases, tending to slow the reaction process down. If the reacting gases are not sufficiently cooled, the concentration of radicals can become high enough to restrict combustion. When the reacting gas is cooled, the radicals recombine to form complex molecules such as  $H_2O$ , and allow the combustion reaction to proceed further towards completion. The formation of complex molecules releases thermal energy into the flow, which is then available for conversion to kinetic energy by the thrust surface [119].

To promote the formation of combustion products, Billig [27] has suggested injecting the fuel at a high equivalence ratio to cool the flame. Another method for promoting the formation of combustion products is to diverge the combustor slightly so that the combustion products are partially expanded and cooled. Diverging the combustor can also have the benefit of increasing the amount of heat that can be released into the flow though combustion before the thermal choking occurs. However, adding heat through an expansion results in a larger decrease in the total pressure and an increase in the heat rejected in the exhaust stream for a given amount of heat released into the flow [111]. Also, if the flow is expanded at too high a rate, the flame may be extinguished and the benefits of expansion will be lost. Therefore, a balance must be achieved for optimum combustor performance.

Another source of thrust loss in the combustor is skin friction, which can become quite high for long combustor ducts. Long combustion ducts also place higher demands on the combustor cooling system. Therefore, there is a need to make the combustor as short as possible. By reducing the length of the combustor, however, the extent to which the combustion reaction runs to completion is also reduced, thereby reducing the chemical energy that is released into the flow. As less chemical energy is released into the flow, the overall engine thrust force will decrease. The amount by which the thrust force will decrease with combustor length, and the amount by which the drag force caused by skin friction will decrease, is highly dependent on the flow conditions within the combustor and the geometry of the combustor. Therefore, it is not a trivial exercise to determine the

#### 4.4 Combustor/Thrust Surface Design

length of the combustor that will give the optimum balance of these opposing forces.

The design of the thrust surface wall contour is equally as important as the design of the combustor duct wall contour. Ideally, the thrust surface contour should expand the exhaust gases to a pressure just above the free-stream pressure so that back flow does not occur. It should also direct the exit flow into a parallel uniform jet aligned with the free-stream. Rao [173] proposed a method for the design of such a contour, however, the method is based on finding an expansion contour for a nozzle of a fixed length using inviscid, non-reacting flow relations. Skin friction and finite-rate recombination processes play an important part in determining the performance of scramjet thrust surfaces, therefore, the Rao method would not be an ideal means of designing the thrust surface. Also, the optimal length of the thrust surface is not known prior to design since it is a function of the thrust surface is to use a flow solver that can model the viscous and reacting mechanisms associated with the flow, and coupling it to a optimization algorithm as in the current study.

### 4.4.2 Design Constraints & Assumptions

The design concept used for the combustor and thrust surface of the axisymmetric scramjet stage is shown in Fig. 4.12. It consisted of a single continuous Bézier curve that



Figure 4.12: Axisymmetric combustor and thrust surface design concept.

makes up the axisymmetric combustor and thrust surface along the centre body of the scramjet, and a straight wall cowl with a 10° expansion at the tip. The contoured combustor and thrust surface were defined with a continuous Bézier curve along the body to give a smooth transition between the duct sections since sharp corners on thrust producing expansion surfaces have been suggested as being detrimental to performance [173]. A Bézier curve was used to define the combustor/thrust surface because they are very versatile in the range of shapes they can produce and the coordinates of the Bézier curve had a radial position that matched the adjoining inlet and the initial slope of the curve was fixed to be parallel to the vehicle centre line. The downstream end of the Bézier curve was also

fixed to be parallel to the centre line and at a radial position to allow for connection to the rocket booster (sting diameter 0.3 m).

The computational domain boundary used for all of the design flow calculations within this section is also shown diagrammatically in Fig. 4.12. Note that the flow calculations excluded the expansion from the cowl tip and assumed that the entire top boundary was a solid no-slip constant temperature wall. The cowl expansion was omitted from the flowfield design calculations since it was assumed that the cowl expansion would not have a significant effect on the thrust surface flow. The position of the cowl expansion and the small thrust contribution from the cowl expansion were considered at the end of the design optimization section where a performance assessment of the optimized design is made.

The left boundary of the computational domain was set as the inflow plane. The flow condition along this plane was taken from the flow conditions calculated at the final downstream plane of the high resolution optimized inlet design discussed in Section 4.3.2. The bottom boundary was set to a no-slip wall at a constant temperature of 1000K and the right boundary was set as the exit plane. Injection of hydrogen fuel was simulated by adding hydrogen though the governing equations source terms across a strip of cells 1 millimetre downstream of the inflow plane (see Fig. 4.13). The strip of cells were centred



**Figure 4.13:** Strip of cells where hydrogen was added to the flow to simulate hydrogen injection from a central strut.

on the midline of the combustor and the strip had a length equal to half the height of the combustor. The hydrogen was injected into the flow through a central strip of cells to simulate fuel injection from a central strut injector. A central strut type injection of the fuel was chosen in preference to a uniform cross-stream injection or a wall injection, to reduce the heat release within the boundary layers through combustion and subsequent wall heat transfer. The position of the fuel injection within the combustor was thought not to have a major influence on the final optimized thrust surface since earlier work associated with this thesis [111] demonstrated that the distribution of heat addition does not effect the profile of the optimized thrust surface significantly. Broadbent has also

observed that the propulsive efficiency is not very sensitive to the precise distribution of heat [32].

The hydrogen fuel was added to the air flow at a fuel rich stoichiometric ratio of 1.3 based on the total mass flow rate of the air within the combustor. This corresponds to a fuel flow rate of 0.398 kg/s. A fuel injection stoichiometric ratio of 1.3 for hydrogen in air has been recommended by Billig [27] as being adequate for cooling purposes at a flight Mach number of 12. Apart from the cooling benefit of a high stoichiometric ratio (or equivalence ratio), a high ratio also limits the maximum temperature in the combustion zone and thereby reduces the fraction of dissociated species in the nozzle expansion which can be a large loss mechanism. The hydrogen was added to the injection region of the flow domain in the simulations through the mass source term in the governing PNS equations (see Eq. 2.5). The amount of hydrogen added to each computational cell within the injection region was calculated by multiplying the density of that cell by a constant. The same constant was used for every cell in the injection region regardless of cell density. The value of the constant was varied until an overall stoichiometric ratio of 1.3 was obtained. The velocity of the injected hydrogen was also set to the velocity of the air in the respective cell, by adding an appropriate momentum source term. Finally, the temperature of the injected hydrogen was set at 800 K which accounts for an expansion of the fuel from the cooling channels. This temperature was set by adding an appropriate energy source term in the governing equations.

# 4.4.3 Parametric Study of Combustor Length

The baseline scramjet combustor/thrust surface design for the combustor length parametric study is shown in Fig. 4.14. The contoured wall of the combustor/thrust surface was defined with a 12 control point Bézier curve. The radial position of the first 8 control



**Figure 4.14:** Layout of Bézier control points which define the contoured surface of the combustor and thrust surface for the combustor length study.

points were set at 0.485 m and the radial position of the remaining control points were set at 0.15 m. The parameter L was varied to give designs with different combustor lengths. Figure 4.14 shows that the length parameter L does not correspond to a constant area combustor section of length L. The Bézier curve produces a slight expansion in the combustor which increases in the downstream direction.

A total of 12 designs were assessed where the length parameter L was set to 0.01, 0.05, 0.1, 0.2, 0.3, 0.5, 0.7, 1.0, 1.5, 2.0, 2.5, and 3.0 metres. The computational domains for each of these design were discretized with 50 cells in the radial direction and from 2000 to 15000 cells in the space-marching axial direction, depending on length. The cells were clustered radially towards the top and bottom of the domain using an exponential clustering parameter of 1.01 (see Eq. 2.104) to match the radial clustering of the inlet computational domain. The cells were also clustered axially towards the inflow plane using a clustering parameter of 1.2.

As stated previously, the inflow conditions for all of the combustor/thrust surface calculations in this chapter, were taken from the final downstream plane of the high resolution optimized inlet design. Figure 4.15 shows the axial velocity profile and static temperature profile for this inflow plane.



**Figure 4.15:** Profile of axial velocity and static temperature for the inflow plane used in the combustor/thrust surface flow calculations.

The top and bottom edges of the domain were set to no-slip constant temperature boundary conditions with a wall temperature of 1000 K. The Baldwin & Lomax turbu-

lence model was used with a compressible damping term to model the development of the boundary layers along these walls (see Section 2.9). A CFL number of 0.25 was used to maintain numerical stability and the convergence criteria was set to a maximum density residual of 0.01%. The modified 8 reaction, 7 species Evans & Schexnayder reaction model was used to model the finite-rate combustion process. The details of this reaction model are presented separately in Appendix C.

The flow calculations (for a single pass of the flow solver over the flow domain) took from 2.7 hours for the short design to 18.5 hours for the long design to complete using one R10000 processor of the SGI Origin 2000. The total calculated axial skin friction drag force, axial thrust force, and heat transfer for each of the combustor/thrust surface designs are presented in Table 4.5. These results are also presented graphically in Fig. 4.16. The

 Table 4.5: Forces and heat transfer calculated for twelve combustor/thrust surface designs with varying length.

Combustor	Combustor/th	rust surfa	ce body forces, kN	Heat
length L, m	Skin friction	Thrust	Net thrust	transfer, MW
0.01	4.1	13.3	9.2	3.8
0.05	4.9	15.9	10.9	4.8
0.1	5.8	17.2	11.4	5.7
0.2	7.6	18.9	11.3	7.9
0.3	9.7	20.2	10.5	10.2
0.5	14.1	22.3	8.2	14.9
0.7	18.0	23.9	5.9	19.4
1.0	23.9	26.0	2.2	26.0
1.5	32.7	36.2	3.5	36.6
2.0	40.3	48.7	8.4	46.1
2.5	47.2	59.6	12.4	55.1
3.0	52.9	68.5	15.6	63.3

results show that the total heat transfer and skin friction tend to increase approximately linearly with combustor length. The total net thrust curve shows an initial peak in thrust for short combustors, a minimum thrust for a design with a L equal to approximately 1 metre, and then a steady rise in total thrust as the combustor length is increased. The behaviour of the thrust performance curve can be explained by considering the finite-rate combustion process of hydrogen and air in a constant area duct. The combustion process begins with an induction period where small concentration of radicals such hydroperoxyl (HO<sub>2</sub>) are formed. In this period, the change in the bulk fluid quantities of the flow do not change appreciably. When the concentration of the induction radicals is high enough, oxidation of hydrogen takes place through a cascade of chain-branching reactions that



Combustor Length Study Results

**Figure 4.16:** Total forces and heat transfer plotted as a function of combustor length for the initial combustor/thrust surface design.

ultimately terminate forming  $H_2O$ . In a constant area duct, the reaction process eventually comes to an equilibrium state down-stream of the reaction front and the reaction process effectively stops. When the reaction process comes to equilibrium, there is no further heat release into the flow. This effect can be seen in the thrust curve shown in Fig. 4.16. There is an initial rapid increase in thrust produced from the combustion process as the combustor length is increased from a very small length, and then the thrust begins to level off up to a design with a combustor length parameter of approximately 1 metre.

As the combustor length is increased, the thrust begins to increase again at approximately a linear rate. The process that is occurring within the combustor that is causing the increase in thrust, is compression of the combustor flow from the boundary layers. The boundary layers continue to grow in thickness as the flow proceeds down the length of the combustor which effectively produces a combustor with converging walls. Therefore, the static pressure of the flow at the start of the expansion is greater than the static pressure that would be generated by combustion alone. The increase in static pressure can be seen in Fig. 4.17 which shows the static pressure as a function of length at a position midway between the top and bottom walls of the combustor/thrust surface. Also shown in this figure, is the static pressure distribution resulting from combustion in a simple constant area duct with slip wall boundary conditions. The simulation for this design used the same inflow conditions and fuel injection specifications that were used for the complete com-



**Figure 4.17:** Midline static pressure distribution for several combustor/thrust surface designs with increasing combustor length. Also shown is the static pressure distribution for 4 metre long, constant area combustor with slip wall conditions.

bustor/thrust surface flow calculations. By setting the wall boundary conditions to a slip wall, the effect of the flow compression from the boundary layer growth is removed and the equilibrium combustion pressure is attained. The static pressure at the inflow plane of the combustor prior to fuel injection is also labelled on the *y*-axis.

The left graph in Fig. 4.17 shows the pressure distribution for the combustor/thrust surface designs with the shorter combustors. For these designs, the maximum static pressure does not reach the equilibrium combustion pressure because of the early expansion. The increase in pressure due to boundary layer compression for these designs is also small compared to the pressure increase due to combustion. In the right graph of Fig. 4.17 are the pressure distributions generated using the designs with the longer combustors, which show the pressure increase due to compression by the boundary layers. The flow compression for the longest design is so great that the pressure increase due to compression is greater than the increase in pressure from the combustion reaction. The pressure fluctuations shown in both graphs are a result of waves generated by a miss-match of static pressure between the fuel injection stream and the rest of the flow.

The total drag force for each design (illustrated in Fig. 4.16) is entirely due to the skin friction acting on the surfaces of the combustor and thrust surfaces. As the length of the combustor increases, the total skin friction increases in an almost linear response (particularly for the shorter designs). This results suggests that the magnitude of the shear stress acting on the walls of the combustor where the majority of the skin friction occurs, is constant. However, the pressure within the combustor steadily increases as the combustor length is increased. Therefore, the shear stress acting on the wall of the pressure within the combustor. A similar result was also obtained recently in an experimental investigation of shock-tunnel skin-friction measurements in a supersonic combustor [72]. That study also showed that the shear stress acting on the walls within a scramjet combustor where combustion did not occur.

The Mach number distributions along a line midway between the top and bottom walls of the combustor and thrust surface are shown in Fig. 4.18 for all of the combustor/thrust surface designs. The right half of the figure shows the Mach number distribution for the



**Figure 4.18:** Midline Mach number distribution for all of the combustor/thrust surface designs. Also shown is the Mach number distribution for a 4 metre long, constant area combustor with slip wall conditions.

designs with the longer combustors where there is a significant amount of flow compression due to boundary layer growth. As the flow is compressed by the boundary layers, the temperature of the flow also increases. This increase in temperature results in an increase in sound speed. Therefore, since the change in flow speed is small, the Mach number of the flow drops as the combustor becomes longer and effectively more narrow. The reduction in Mach number for the longest combustor design is so great the entire flow almost becomes subsonic. A design having a longer combustor would probably result in the combustor becoming choked. The Mach number of the centre line flow at the inflow plane is also marked on the graphs in Fig. 4.18. There is a rapid decrease in the Mach number from this initial value as soon as the fuel is injected into the flow. Hydrogen has a much lower molecular mass than the average molecular mass of air. Subsequently, when hydrogen is introduced into the flow, the sound speed of the gas mixture increases and the Mach number reduces.

The final part of the combustor/thrust surface design assessment for the various combustor lengths was an analysis of the chemical species formed and consumed through the combustion process. The distribution of  $H_2$ , H, OH and  $H_2O$  along a line mid-way between the contoured surface and the cowl for all of the designs is shown in Fig. 4.19.



Figure 4.19: Midline mass fractions for several combustor/thrust surface designs with increasing combustor length.

The mass fraction plots reveal several interesting points regarding the combustion process and how it is effected by the length of the combustor duct :

• The ignition delay time for the combustor/thrust surface design with the shortest combustor, L = 0.01m, was substantially increased due to expansion waves cooling the air/fuel mixture prior to the combustion front. The short combustor also caused the recombination of the excess unburnt hydrogen to become frozen very rapidly. This can be seen in the mass fraction plots for molecular hydrogen and atomic hydrogen. Since there is a relatively high concentration of atomic hydrogen in the exit flow of the short combustor, a considerable amount of energy is lost in the exhaust flow through the unrecombined hydrogen atoms.

• The H, OH and  $H_2O$  mass fraction plots for the long combustor designs show that  $H_2O$  formed as a result of combustion is dissociated as the flow is compressed by the growing boundary layers. The boundary layers raise the mean temperature of the flow and cause some of the  $H_2O$  molecules to dissociate. However, the expansion following the combustor is gradual enough to allow all of the dissociated  $H_2O$  to recombine before exiting the scramjet. If the expansion was more rapid, the recombination process may freeze and energy could be lost as dissociated radicals, such as H and OH.

• The centre line  $H_2O$  mass fraction at the exit plane of the scramjet for all of the designs are very similar. This result indicates that the expansion rate of the thrust surfaces for all of the designs was slow enough to ensure that the recombination reactions for the radicals involved in the combustion reaction, did not freeze. However, as discussed previously, the recombination reactions for the excess atomic hydrogen to molecular hydrogen do become frozen for the shorter combustors.

The combustor/thrust surface design with a combustor length parameter of 0.1 metres was selected as the initial design to be optimized using the Nelder-Mead optimization algorithm. This design exhibited a high net thrust while having a low overall heat transfer. The designs with very long combustors (L = 2.5 & 3.0) gave greater thrusts, however, the heat transfer through the walls was an order of magnitude greater. Clearly the combustor/thrust surface designs with the shorter combustors are superior to the long combustor designs (neglecting mixing). It is important to realise that this distinction may not have been identified if the parametric study had not been performed prior to solving the design optimization problem using the Nelder-Mead optimization algorithm. The Nelder-Mead optimization algorithm is a sloped-based optimizer and the objective function was only a function of the overall thrust and did not contain any term relating to the heat transfer associated with a particular design. Therefore, the optimization algorithm may have converged to a design solution with a very long combustor if the initial design had a combustor with a large length to start with. If this was the case, the benefits of reducing the combustor length may not have been realised. By starting with an initial design with a

short combustor, the likelihood of the optimizer converging to an optimal design with a short combustor length and low heat transfer becomes greater.

# 4.4.4 Optimization of Combustor and Thrust Surface

The optimization problem for the combustor and thrust surface consisted of optimizing the geometry of an initial design for maximum axial thrust. The geometry of the combustor/thrust surface was defined with six design variables that specified the length of the combustor, the length of the thrust surface, and the shape of the thrust surface Bézier curve (see Fig. 4.20). The Bézier curve was defined with 12 control points where the



Figure 4.20: Design variables for optimization of combustor/thrust surface.

radial position of the first six upstream control points were fixed as were the radial position of the last two downstream control points. The axial position of the Bézier control points were set as functions of the length design variables, dv[0] and dv[1], and the radial position of the four unconstrained control points were used as design variables, dv[2] to dv[5]. The radial positions of the six upstream control points were constrained primarily to prevent the optimizer from attempting to converge the combustor duct. However, as was shown in the parametric study, this constraint does not prevent the Bézier curve from forming a combustor with a diverging wall since the neighbouring downstream control points have a strong influence on the combustor wall slope when the combustor length design variable, dv[0], is small. The radial constraint on the last two downstream control points was imposed to maintain curvature continuity with the mating connector sting.

A further constraint was also imposed on the maximum radial position of the design control points, dv[2] to dv[5], to prevent the Bézier curve from having a radial position

greater than the radial position of the first six upstream control points. This constraint was imposed by first assessing the radial position of all points along a prospective Bézier curve design determined by the optimizer before the design was issued to the flow solver. If any part of the curve had a radial coordinate greater than the limit, the nearest Bézier control point was reduced until the curve was acceptable. The modified design was then given to the flow solver. If this constraint had not been used, the optimizer may have attempted to converge the duct in order to increase the flow temperature and burn the fuel subsonically.

The initial values of the design variables and the initial perturbations (in metres) for all of the design variables are given in Table 4.6.

**Table 4.6:** Initial design variables and perturbations for the combustor/thrust surface optimization (in metres).

Design variable	dv[0]	dv[1]	dv[2]	dv[3]	dv[4]	dv[5]
Initial values	0.1	1.0	0.4851	0.4851	0.15	0.15
Initial perturbations	0.05	0.5	-0.15	-0.15	0.15	0.15

The computational setup used for the optimization flow calculations was the same as the setup used for the parametric combustor length study discussed earlier. A computational domain discretization of  $50 \times 2000$  cells was used for all of the flow calculation regardless of combustor and thrust surface length.

The objective function for the optimization problem was set as the summation of an arbitrary force value of 50 kN and the integrated total combustor/thrust surface thrust force calculated by the flow solver due to pressure and friction (where axial thrust is negative for a propulsive force). This formulation of the objective function was used to ensure that a design with a high propulsive thrust results in a low positive objective function evaluation. The Nelder-Mead optimization algorithm was used to minimise this objective function by perturbing the initial design variables. A simplex variance of 10 Newtons was set as the optimization convergence criteria (see Eq. 3.1).

The results of the combustor/thrust surface optimization are shown if Fig. 4.21 where the total calculated thrust for each design is plotted against the design iteration (a negative value indicates a propulsive thrust). The optimization record shows that an optimum design was first found after 126 evaluations of the objective function (with one flow solution computed per function evaluation). The variance of the simplex after 126 evaluations (or iterations) was approximately 50 N so the optimization algorithm continued to search for an improved design. In subsequent iterations, no improvement could be made to this



Figure 4.21: Optimization record for the combustor/thrust surface showing total thrust in kN.

design and the simplex variance maintained a value of approximately 50 N. Therefore, the optimization algorithm was manually stopped after 158 iterations where it had become clear that the simplex variance was not going to decrease substantially with further searching. The variance of 50 N may have been a result of the reflecting waves generated by the miss-match of static pressure between the fuel injection stream and the rest of the flow (as discussed previously).

The net result of the optimization was an increase in axial thrust developed by the combustor/thrust surface from an initial value of 11.36 kN to 13.52 kN which is a substantial 19% increase. The initial and optimized design variables are shown in Table 4.7. The optimization algorithm took 290.1 CPU hours (using one R10000 processor of the

Table 4.7: Initial and optimized design variables for the combustor/thrust surface.

Design variable	dv[0]	dv[1]	dv[2]	dv[3]	dv[4]	dv[5]
Initial values	0.1	1.0	0.4851	0.4851	0.15	0.15
Optimum values	0.2344	1.1656	0.3304	0.3222	0.0856	0.2975

SGI Origin 2000) to complete the 126 objective function evaluations required to optimize the combustor/thrust surface design.

The optimized combustor/thrust surface design for the Mach 12 axisymmetric scramjet is compared against the initial design and a straight ramp expansion design in the contour plots shown in Figs. 4.22 and 4.23. The plots show contours of static pressure and Mach number for all three designs.



**Figure 4.22:** Contour plots of static pressure for the initial, optimized and straight wall combustor/thrust surface designs (the contour intervals are distributed over a  $\log_{10}$  scale).



Figure 4.23: Contour plots of Mach number for the initial, optimized and straight wall combustor/thrust surface designs.

The straight ramp combustor/thrust surface design is the same length as the optimized design and the start of the expansion is positioned at the same axial position where the duct height of the optimized design is 10% greater than the initial combustor duct height. Therefore, the combustor length is very similar to the optimized combustor length. This can be seen in Fig. 4.24 which shows the wall profiles for all three designs. This figure



Figure 4.24: Profiles of wall designs for the combustor/thrust surface.

also shows that the upstream geometry of the initial design and the optimized design are very similar.

The calculated forces and heat transfers associated which each of the three designs are listed in Table 4.8. The exerted drag force (due entirely to skin friction) and heat transfer

**Table 4.8:** Forces exerted on the combustor/thrust surface designs in kN and total heat transfer through the internal walls in MW.

Design	Drag	Thrust	Net Thrust	Heat transfer
Initial	5.83	17.19	11.36	5.75
Optimized	5.95	19.47	13.52	5.93
Straight	5.93	19.17	13.24	5.92

for each of the three designs is very similar despite the difference in geometry. However, there is a large difference in net thrust between the initial design and the optimized design. Most of the net thrust difference between the initial design and the optimized design is a result of the increased force on the thrust surface rather than a decrease in drag from skin friction. It is also interesting to note that the net thrust for the straight ramp design is similar to the net thrust for the optimized design. This result indicates that the thrust developed is more sensitive to the overall rate of expansion (or length for a fixed expansion ratio) than the contour of the expansion. This is consistent with the study by Jacobs &

Craddock [111] where most of the benefit gained for an inviscid optimization of a scramjet nozzle came from lengthening the expansion surface.

The optimized thrust surface and the straight ramp thrust surface design both maintain a higher pressure across the thrust surface over a larger radial distance which translates to a higher overall thrust. This can be seen in Fig. 4.25 which shows the static pressure along the thrust surface as a function of radial distance. The good thrust performance of



Figure 4.25: The radial distribution of static pressure over the three thrust surfaces designs.

the straight ramp expansion design is due to the high pressure at the start of the expansion where the radial wall coordinate is large. Axisymmetric designs with high propulsive pressures at large radial distances are advantageous because of the increased circumferential area.

Even though the contoured optimized design and the straight ramp design have very similar net thrusts, the contoured design is favoured because the contoured expansion generates an exhaust flow that is more aligned to the axis of the vehicle. Axial exhaust flow may result in a lower form drag for any downstream aerodynamic surfaces compared to the drag that would result from flow that is turned into the axis. Also, the static pressure at the downstream end of the internal cowl surface is lower for the contoured thrust surface design compared to the straight ramp thrust surface (see Fig. 4.22). Therefore, the cowl tip would need to be positioned further downstream for the straight ramp expansion design to ensure the tip pressure would not cause flow reversal. The longer cowl would result in a higher skin friction drag force.

The similar total drag and heat transfer for all three designs is predominately a result of the designs having approximately the same combustor length (in terms of a constant area length). The levels of skin friction and heat transfer on the combustor walls are much greater than the those seen on the expansion surfaces. Therefore, since the combustor skin friction and heat transfer distribution are similar for all three designs, the total skin friction and heat transfer for the three designs are also similar. The distribution of skin friction and heat transfer for the three designs is illustrated in Fig. 4.26 which shows the calculated axial skin friction and heat transfer distribution per metre length for all three designs (note that this includes the skin friction and heat transfer from the internal cowl surface also). These figures show the very high skin friction and heat transfer within the



Figure 4.26: Rate of skin friction and heat transfer along length of the three combustor/thrust surface designs.

combustor region and a rapid decrease in the levels as the flow is expanded.

The extent to which the combustion reaction proceeds to the equilibrium state within the combustor for the three combustor/thrust surface designs, can be determined from the midline static pressure and temperature plots in Fig. 4.27. These plots show the pressure and temperature along a line midway between the top and bottom surfaces of the combustor/thrust surface designs. Also shown on these plots are the pressure and temperature distributions for a constant area combustor where the wall conditions have been set to a slip wall so that boundary layer growth is omitted from the calculations (and thus flow compression from the boundary layer). The constant area distributions give an approximation of the final equilibrium pressure and temperature of the combustion reaction. A



**Figure 4.27:** Midline static pressure and temperature distribution for the initial, optimized and straight ramp combustor/thrust surface designs. Also shown are the distributions for a 1.4 metre constant area combustor with slip wall conditions.

comparison of the constant area combustor results with the other combustor/thrust surface results shows that the amount of chemical energy released into the flow for the three combustor/thrust surface designs, is significantly lower than the maximum possible chemical energy attainable by running the combustion reaction to an equilibrium state. The reduction in the amount of chemical energy release is a result of the short combustor length. However, the loss of chemical energy is balanced by a reduction in the combustor skin friction due to the short combustor lengths.

The calculated distributions of  $H_2$ , H, OH and  $H_2O$  mass fractions along a line midway between the top and bottom surfaces of the combustor/thrust surface designs are shown in Fig. 4.28. The mass fraction distributions are similar for all the combustor/thrust surface designs which would indicate that the combustor and upstream section of the thrust surfaces are similar in design. The  $H_2$  and H plots show that the hydrogen recombination process freezes at the early stages of the expansion. Subsequently, the contour of the remaining section of the thrust surface would have little effect on the recombination process for hydrogen. Also, the recombination of the  $H_2O$  water molecules is almost completed in the upstream section of the thrust surface. The completion of the recombination process is indicated by the plateauing of the  $H_2O$  mass fraction distribution and the consumption of most of the OH molecules. Therefore, the contour of the downstream thrust surface has little effect on the amount of chemical energy released into the flow. This result was to be expected because of the lower static temperatures and the higher speed of the flow across the downstream section of the thrust surface.

The distribution of midline static pressure and the mass fraction plots for the initial, optimized and straight ramp combustor/thrust surface designs, indicate that the amount of chemical energy extracted out of the combustion process was very similar for all three designs. Therefore, it can be concluded that most of the improvement in thrust performance between the initial design and the optimized design was obtained by contouring and lengthening the thrust surface so that a high pressure is maintained on the thrust sur-


Figure 4.28: Mass fraction distributions for the initial, optimized and straight ramp combustor/thrust surface designs.

face over a greater radial distance.

To compete the optimized combustor/thrust surface design, a cowl lip with a  $10^{\circ}$  expansion was added. The cowl lip expansion was added to the top wall of the optimized design at an axial position where the static pressure at the cowl tip would be greater than the external cowl static pressure and less than a pressure 500 Pa greater than the external cowl static pressure. This design condition was imposed to ensure that reverse flow would not occur on either the cowl lip expansion or the external cowl surface [22]. The external cowl static pressure was approximated as 1300 Pa using the flow data from the cowl simulations performed for the inlet design (see Section 4.3.2). Several trial simulations were required in order to find a suitable position for the cowl expansion. In all of these simulations, the top boundary of the computational domain was changed to a uniform supersonic inflow and the flow around the exterior of the scramjet. The angle of the supersonic inflow domain boundary was large enough to accommodate the expansion fan emanating from the cowl tip. The uniform supersonic inflow domain boundary condition downstream of

the cowl tip was set to:

$$P = 1300 \text{ Pa}, \quad T = 340 \text{ K},$$
  
 $\rho = 0.012 \text{ kg/m}^3, \text{ and } u = 3634 \text{ m/s},$ 

This flow condition was taken from the cowl simulation in Section 4.3.2 and is similar to the free-stream flow condition. The Mach number and static pressure contours from the flow solution of the optimized combustor/thrust surface design with the cowl expansion are shown in Fig. 4.29. The contour plots were generated with the same contour levels



**Figure 4.29:** Mach contours and static pressure contours for the optimized combustor/thrust surface design with the leeward cowl tip expansion.

used for the plots in Figs. 4.22 and 4.23. A comparison of the two sets of plots for the optimized design shows that the cowl expansion does not effect the thrust surface pressure distribution. Therefore, the assumption made for the optimization flow calculations was valid.

The thrust contribution from the cowl expansion can be determined by assessing the difference in the overall calculated thrust for the optimized design with and without the cowl expansion. The total calculated forces and heat transfer for both designs are listed in Table 4.9. The overall gain in net thrust from the cowl tip expansion is 0.26 kN which is only a 1.9% increase in the total thrust. Of this gain in thrust, 0.09 kN was due to a reduction skin friction because of the reduced cowl length, and 0.17 kN was due to the static pressure on the cowl expansion. The reduction in heat transfer was also minimal at 0.08 MW (1.3%).

Design	Drag	Thrust	Net Thrust	Heat transfer
Without cowl expansion	5.95	19.47	13.52	5.93
With cowl expansion	5.86	19.64	13.78	5.85

**Table 4.9:** Forces exerted on the optimized combustor/thrust surface designs in kN and total heat transfer through the internal walls in MW.

## 4.5 Grid Refinement Study

This section presents a grid refinement study that was carried out for the optimized inlet, combustor/thrust surface and external cowl computational solutions to ensure that the computational flow solutions presented in this chapter converge to an exact solution for an increasing grid resolution. By "exact solution" it is meant the solution that would be generated by the flow solver using a computational domain disctretized with cells of infinitesimal size and by convergence, it is meant that the approximate solution to the PNS equations approaches the exact solution for the same initial and boundary conditions as the computational grid is refined. The accuracy of the computational scheme is not under question in this analysis since it has been treated separately in Appendix E.

Each of the grid refinement studies used a set of four grids with 20, 40, 80 and 160 cells in the cross-stream direction to discretize the computational domains. This gives a grid refinement ratio of 2 if the axial grid resolution is scaled using the same ratio for each of the four grids. The high resolution flow calculations used for the design of the scramjet, all used 50 cells in the cross-stream direction which is a grid resolution that was not part of the refinement set. Therefore, the high resolution design flow calculations provide a secondary data point for the refinement studies to ensure convergence.

The total calculated axial force was used to determine the order of convergence and solution error for each of the refinement studies since the axial force is an important quantity used for analysis in this chapter. The total axial force was calculated by summing the axial components of the integrated static pressure and viscous stress for all of the wetted surfaces. The order of convergence for the solution scheme, p, can be approximately determined using the relation,

$$p = \ln\left(\frac{f_1 - f_2}{f_2 - f_3}\right) / \ln(r)$$
(4.8)

where  $f_1$ ,  $f_2$  and  $f_3$  are the axial forces of the discrete solution for increasing grid resolutions and r is the grid refinement ratio (which in this case is 2). Also, an estimate of the fractional error in the calculated axial force can be determined using a generalised version of Richardson extrapolation [180]. The estimated fractional error, E, is given as

$$E_2 = \epsilon/(r^p - 1) \tag{4.9}$$

where

$$\epsilon = (f_1 - f_2)/f_2 \quad . \tag{4.10}$$

The error,  $E_2$ , is an ordered approximation to the actual fractional error of the quantity  $f_2$ .

A grid refinement study was first performed for the optimized inlet design using a set of four grids of increasing resolution where each grid was clustered with the same clustering parameters used for the design optimization grids (see Section 4.3.2). The same boundary conditions, computational flow models and numerical stability and convergence criteria were also used for the refinement calculations. Table 4.10 lists the number of radial grid cells, top and bottom wall  $y^+$  values at the exit plane, and total calculated axial drag for each of the inlet flow calculations. Also shown for comparison are the results from the design calculations.

**Table 4.10:** Total calculated drag force (in kN) exerted on the optimized inlet design for grids of increasing resolution.

No. of radial	No. of axial	Top y <sup>+</sup>	Bottom y <sup>+</sup>	Total drag
cells	cells	wall value	wall value	force, kN
20	5000	11.2	10.7	12.43
40	10000	6.0	5.7	13.25
80	20000	3.5	3.1	13.86
160	40000	1.9	1.6	14.17
50	10000	5.2	4.7	13.45

The tabulated exit plane  $y^+$  values for the cells nearest the wall are not the highest  $y^+$  wall values for the simulations. The wall  $y^+$  values actually peak at the upstream tip of the inlet and decrease to the quoted values at the inlet exit plane as illustrated in Fig. 4.30 for the simulation with 80 radial cells (where the exit plane of the inlet is at x = 1.91 m). Also shown in this figure is the axial distribution of skin friction force per unit length. A comparison between the two plots in the figure shows that the contribution to wall skin friction force from the upstream section of the inlet where the wall  $y^+$  values are greatest, is small relative to the contribution of skin friction force from the combustor region. Therefore, the quoted  $y^+$  values in Table 4.10 represent wall  $y^+$  values in the flow regions where the majority of the skin friction force is contributed and are more significant than the maximum wall  $y^+$  value (in terms of skin friction error).



**Figure 4.30:** Axial distribution of (a) wall  $y^+$  values and (b) wall axial skin friction per unit metre for the scramjet simulations with 80 radial cells.

Evaluating the convergence order expression given in Eq. 4.8 using the axial force calculated from the flow solutions for the three lowest resolution grids gives a convergence order of 0.43, and for the highest three resolutions an order of 0.98. The convergence order for the three highest resolution grids is very close to the nominal convergence order of the flow solver which is approximately 1.0. The reason for the poor convergence order for the first three computational solutions was believed to be the inadequate resolution of the turbulent boundary layers. The wall  $y^+$  values for the lowest resolution simulation are quite high for a turbulent boundary layer simulation. Nevertheless, the positive and increasing convergence order indicates that the computational solutions will converge to an exact solution as the grid resolution is increased.

The approximated fractional error in axial drag force given by Eq. 4.9 for the high resolution inlet solution is 2.2%. Therefore, an approximation of the exact (that is the exact solution of the PNS equations) drag force sustained by the inlet is 14.47 kN.

The grid refinement study for the optimized combustor/thrust surface design was performed once for a flow without any fuel injection and then again with fuel injection. The flow calculations performed with and without fuel injection all used the same grid clustering parameters, boundary conditions, computational flow models and numerical stability and convergence criteria that were used for the design calculations in Section 4.4. The calculated total axial thrusts for the four combustor/thrust surface grid refinement simulations and the design simulation without fuel injection are presented in Table 4.11. The  $y^+$ 

No. of radial	No. of axial	Top y <sup>+</sup>	Bottom y <sup>+</sup>	Total thrust
cells	cells	wall value	wall value	force, kN
20	2000	12.7	11.1	4.83
40	4000	7.1	6.1	4.50
80	8000	4.3	3.5	4.25
160	16000	2.6	1.9	4.12
50	4000	6.1	5.0	4.39

**Table 4.11:** Total calculated thrust force (in kN) exerted on the optimized combustor/thrust surface design for grids of increasing resolution – no fuel.

values quoted in the above table are the maximum wall values in the combustor region. The wall  $y^+$  values fall off from these peak values moving downstream into the expansion, then begin to rise as the grid resolution becomes coarser with the widening duct (see Fig. 4.30). The wall  $y^+$  values at the exit flow plane are slightly greater than those quoted in the table, however, the contribution to drag is small on the downstream thrust surfaces in comparison to the drag on the combustor surfaces.

The convergence order for the three lowest resolution grids is 0.40 and the order for highest three grids is 0.94. Not surprisingly, these convergence orders are similar to the convergence orders for the inlet grid refinement study. For the same reasoning given previously, these convergence orders indicate that the computational solutions will converge to an exact solution as the grid resolution is increased. The approximated fractional error in axial thrust force for the high resolution combustor/thrust surface calculated using the generalised version of Richardson extrapolation is 3.4%. The estimation of the exact thrust force developed by the optimized combustor/thrust surface with no fuel injection is therefore 3.98kN.

The calculated total axial thrusts for the four combustor/thrust surface grid refinement simulations and the design simulation with fuel injection are presented in Table 4.12. The convergence order for the three lowest resolution grids is 0.28 and the order for highest three grids is 0.42. Both convergence orders are well below the nominal value of 1.0. The low convergence rates were believed to be a result of the method used to inject the fuel into the flow. As stated previously in Section 4.4.2, the rate of hydrogen addition for each computational cell within the injection zone was calculated by multiplying the density of that cell by a constant. The same constant was used for every cell in the injection zone regardless of cell density.

No. of radial	No. of axial	Top $y^+$	Bottom y <sup>+</sup>	Total thrust
cells	cells	wall value	wall value	force, kN
20	2000	19.0	17.1	16.08
40	4000	11.4	9.8	14.36
80	8000	6.6	5.6	12.94
160	16000	3.9	2.9	11.88
50	4000	8.7	7.9	13.78

**Table 4.12:** Total calculated thrust force (in kN) exerted on the optimized combustor/thrust surface design for grids of increasing resolution.

stoichiometric ratio of 1.3 was obtained. In order to maintain the same stoichiometric ratio for all the grid refinement flow calculations, a different constant had to be used for each grid resolution. A different constant had to be used because the inflow property distributions differed slightly for each grid resolution. The variation in density distribution for all of the inflow planes used for the refinement study can be seen in Fig. 4.31. These



Figure 4.31: The density distributions across the inflow plane for the combustor/thrust surface grid refinement study.

distributions were obtained from the exit plane of the inlet grid refinement calculations. The figure shows that there is a substantial difference in density distribution across the inflow plane particularly in the injection zone. A similar variation also occurs for the other conserved flow properties. The consequence of this variation is a different distribution of mass, momentum and energy addition across the injection zone for each of the grid resolution calculations. This difference was believed to result in the poor convergence rates since the convergence rates without fuel addition were close to nominal. It would be

wise to adopt a different injection strategy in future computational studies for this reason.

An estimation of the error for the high resolution flow calculation with fuel addition was not made because it would be a meaningless value since the fuel injection was not consistent between simulations.

The last grid refinement study performed was for flow simulations of the entire length of the external cowl. Up to this point, the external cowl flow-field had only been simulated up to the axial point marking the exit plane of the inlet since the entire length of the cowl was not known prior to the optimization of the combustor/thrust surface. The computational setup for the complete cowl simulations was the same as the setup used for the cowl simulations performed previously in Section 4.3.2. The computational domain for the grid refinement calculations started at the upstream tip of the bent cowl and finished at the downstream tip of the cowl expansion. The bottom boundary of the computational domain was bound by the external cowl, and the top boundary was angled to include the shock emanating from the upwind bent cowl section. A clustering parameter of 1.02 was used to cluster the grids towards the cowl surface and a clustering parameter of 1.1 was also used to cluster the grids towards the inflow plane. The bottom boundary condition was set to a no-slip, constant temperature wall at 1000 K, and the top boundary was set to a supersonic inflow condition (the inflow conditions are listed in Section 4.3.2). A turbulent boundary layer was assumed to develop from the cowl leading edge. The gas was modelled with the same non-reacting thermodynamic equilibrium model used for the inlet calculations. Numerical stability was maintained using a CFL number of 0.45 and the numerical convergence criteria was set at a density residual of 0.01%.

The calculated total axial drag force for the four grid refinement cowl simulations are presented in Table 4.13. Also shown in this table are the dimensions of the grid used for each simulation and the  $y^+$  value for the cell nearest the wall at the end of the cowl. The convergence orders for the cowl simulations were very close to the nominal convergence rate at 0.93 for the three lowest resolution simulations and 0.99 for the three highest

No. of radial	No. of axial	South y <sup>+</sup>	Total thrust
cells	cells	wall value	force, kN
20	5000	6.9	4.397
40	10000	3.9	4.612
80	20000	2.1	4.725
160	40000	1.2	4.782

**Table 4.13:** Total calculated drag force (in kN) exerted on the external cowl surface design for grids of increasing resolution.

resolution simulations. The extrapolated fractional error in drag for the highest resolution simulation is 1.2% and the estimated exact axial drag force on the cowl is 4.840 kN.

The grid refinement studies discussed in this section demonstrated that the flow calculations performed in this chapter for the scramjet design optimization will all converge if the grid resolution is increased. As expected, the results of the grid refinement studies also showed that the accuracy of the flow calculations is strongly dependent on the how accurately the turbulent boundary layers are resolved. In order to obtain a solution error for axial force on the order of a few percent, it was necessary to cluster the grid so that the cell closest to the wall has a  $y^+$  value is on the order of 1. This is an important result to consider when performing scramjet optimization studies where the drag force due to skin friction is of the same order as the thrust developed by combustion.

## 4.6 Complete Optimized Engine Analysis

The Mach contours and static pressure contours for the complete optimized Mach 12 axisymmetric scramjet engine flow-field are shown in Fig. 4.32. Also shown in this figure



**Figure 4.32:** Contour plots of Mach number and static pressure for the flow-field generated by the complete optimized scramjet design.

are the boundaries of the computational domains used to perform the flow calculations as well as the Mach number and static pressure at selected positions within the flow-field. The contour plots were constructed from the grid refinement flow solutions that used 80 cells in the cross-stream direction to discretize the computational domains (see previous section). An overall listing of the axial forces applied to the engine components is given in Table 4.14 where the forces are listed in kN and a positive force indicates a thrust force. The forces listed were calculated from the high resolution flow solutions used for

		Initial			(	Optimized	
	Inviscid	Viscous	Total	. –	Inviscid	Viscous	Total
Inlet	-10.95	-5.02	-15.97		-8.79	-4.66	-13.45
Nozzle	17.21	-5.83	11.38		19.64	-5.86	13.78
Cowl	-4.80	-1.15	-5.95		-3.52	-1.03	-4.55
Total	1.46	-12.00	-10.54		7.33	-11.55	-4.22

**Table 4.14:** Overall listing of the calculated axial forces (in kN) applied to the engine components.Positive force indicates thrust, negative force indicates drag.

design. The grids for these flow solutions contained 50 cells in the radial direction. A separate high resolution flow calculation had to be undertaken for the initial cowl design which included the complete length of the cowl. The forces listed for the initial design of the combustor/thrust surface (listed as Nozzle in the table for brevity) were taken from the high resolution flow solution that did not include a cowl lip expansion. A cowl lip expansion was not included because the static pressure distribution on the internal side of the cowl necessitates positioning the start of the cowl tip expansion at the very end of the cowl length. Therefore, no reduction in skin friction drag would be obtained by modelling a cowl tip expansion. Also, the gain in propulsive thrust force by including the expansion would have been negligible (see gain in force for optimized design in Table 4.9).

The total axial force exerted on the optimized scramjet engine is shown to be a drag force, thus indicating that the engine design does not produce a propulsive thrust. This was not a surprising result considering the large amount of skin friction that was present in the engine. It should also be expected that this calculated total force would be, at best, as an optimistic value of the drag force. In reality, the engine would experience a greater drag force because of several additional design changes that would have to be made for the real engine. Some possible design changes that may contribute to the drag are as follows:

(1) A fuel injection system would have to be included in the real engine design since in this study, the hydrogen fuel was simply introduced into the flow through the source terms in the governing equations used to model the flow. Therefore, the predictions of axial force for the engine did not include a drag force attributed to injectors which would be considerably high if placed within the combustor flow-field. A better option for high Mach number flow may be to use port hole injectors on the inlet surfaces or step injectors on the sides of the combustor walls. Upstream port hole fuel injection consists of

#### 4.6 Complete Optimized Engine Analysis

injecting fuel through orifices on the walls of the inlet so that a jet of fuel penetrates the inlet boundary layer and into the core flow. The fuel then mixes with the air as it travels through the inlet thus eliminating the need for an excessively long combustor to undertake fuel mixing. Wall fuel injection through a rearward facing step or slot around the circumference of the combustor, reduces combustor skin friction and heat transfer by displacing the high temperature boundary layer and replacing it with a cooler layer of fuel.

(2) The combustor length would have to be substantially longer than the optimized combustor designed in this study. The modelling of the flow through the combustor assumed that the fuel was introduced into the flow perfectly mixed with the air. In a real engine design, the injected fuel would require time to adequately mix with the air through turbulent mixing processes and diffusion. The longer the combustor, the more time the fuel has to mix with the air. However, the drag due to skin friction increases substantially with combustor length as was discussed in Section 4.4.

(3) An axisymmetric scramjet configuration may require flow fences or walls on the radial planes within the combustor to provide differential thrust control. For a "wrap-around" axisymmetric engine at an angle of attack, the air will tend to move around to the leeward side of the engine if it is not constrained. Therefore, the performance of the windward side of the engine will be significantly reduced because of reduced mass flow rate which may result in an unfavourable torque on the engine. Introducing flow fences may alleviate this problem, however, a substantial gain in skin friction drag would be incurred due to the extra wetted surface area.

Despite the poor overall thrust performance of the optimized design, the overall reduction in drag through optimization was considerable. The 10.54 kN drag force of the initial design was reduced by 6.32 kN through optimization (based on the high resolution design calculations). This improvement in performance was attained through only small changes to the initial design. The overall design concept remained unchanged because of the geometrical constraints used during optimization. The magnitude of the geometric changes made to the initial design can be seen in Fig. 4.33 which shows the wall profile of the initial and optimized designs. Even though the optimization results indicate scramjet design optimization is worthwhile, the fact that small changes in design can make such a large difference to the net thrust of the scramjet is of some concern. The sensitivity of the net thrust to the design seems to come from the *thrust – drag* calculation which is the difference between two similar forces. If such a sensitivity exists for the geometrical design of a scramjet, a similar sensitivity may exist for the flight condition and the angle of attack. These sensitivities were not explored in this study but do warrant further investigation.

The total skin friction calculated for the optimized scramjet design was almost as great as the form drag due to static pressure. This result indicates that modelling skin



Figure 4.33: Wall profiles of the initial and optimized axisymmetric scramjet designs.

friction is vital to the accurate prediction of scramjet performance, particularly for high flight Mach numbers where the temperatures and pressures associated with the scramjet combustor can drive the skin friction to excessive levels. A purely inviscid flow analysis of the optimized engine design would falsely conclude that the engine would produce a positive thrust.

Another interesting result with regard to the total calculated skin friction is the small difference in total skin friction between the initial design and the optimized design. Most of the improvement in performance resulted from the minimisation of form drag (or drag due to static pressure) and the improvement in the thrust surface contour rather than skin friction reduction. The reason why the skin friction is so similar between the initial and optimized designs, was thought to be a result of the two designs having very similar combustor lengths since the majority of the engine skin friction is due to the combustor surfaces.

Overall, the optimization algorithm was responsible for a substantial improvement in thrust performance of the initial design. In this case, the improvement was not great enough to make the design suitable for an actual flight vehicle. The major failing of the design was thought to be the excessive skin friction resulting from the wrap around design concept. As discussed at the end of Section 4.3.3, a cylindrical type combustor resulting from a funnel type inlet would have approximately 8 times less surface area than the combustor concept used in this study. If the average skin friction level for the combustor designed in the current study is assumed to be 17.5 kN per metre length of the combustor (see Figs. 4.10 & 4.26), and the combustor length is approximately 0.2 metres (see Fig. 4.33), then the contribution of skin friction from the combustor is approximately 3.5 kN. Further, if it is also assumed that a scramjet design with a funnel type inlet and cylindrical combustor experiences the same wall shear stress within the combustor as calculated for the combustor in this study, then the reduction in combustor skin friction would be approximately 3.06 kN which is a very substantial amount. Therefore, it would be advisable for future designers of scramjet engines to employ design concepts that minimise the wetted surface area of the combustor.

### 4.7 Summary & Recommendations

A computational design tool consisting of a Nelder-Mead optimization algorithm and an efficient compressible flow solver was successfully used to significantly improve the performance of an axisymmetric Mach 12 scramjet design. The improvement in performance was made through small geometric changes to the initial design, which resulted in improvements to the inviscid drag and thrust forces rather than significant reductions in skin friction. The computational scramjet design study was undertaken in two separate stages, where the inlet was designed independently of the combustor/thrust surface. The calculated exit flow from the final inlet design was used as the inflow condition for all of the design calculations for the combustor/thrust surface. The initial designs for the inlet and the combustor/thrust surface were obtained through analysis and parametric studies conducted prior to optimization to ensure that the designs were close to their optimal design. This approach was taken to improve the effectiveness of the Nelder-Mead optimization algorithm since it is a slope-based algorithm that is more effective in the local design space.

The inlet design was undertaken by assessing a short, long, and bent cowl inlet design, where the bent cowl inlet design was optimized for minimum drag. All three inlets were designed for the same mass capture area and core flow exit temperature. The bent cowl inlet was selected as the inlet to be used in the final scramjet design since it had a low drag and was less likely to be prone to boundary layer separation due to rapid increases in pressure from shock waves. The optimization results of the bent cowl inlet showed that an inlet optimized for minimum drag cancels shocks at expansion corners. Subsequently, the optimized design produced shock free flow leading into the combustor. The drag associated with the bent cowl inlet was reduced by 17% through optimization of the inlet geometry.

The design of the combustor/thrust surface was also carried out through a process of analysis and optimization. The analysis consisted of a parametric study of combustor length for an initial constant area combustor/thrust surface design. The combustion process within each design was modelled using an efficient finite-rate chemical reaction model, which was developed and optimized for the conditions studied (see Appendix C). The results of the parametric study showed that a peak in thrust performance occurs for a combustor length substantially shorter than the length required for the combustion reaction to come to an equilibrium state. The reduced length resulted in a loss of available chemical energy since the combustion reaction was retarded by an early expansion that cooled the flow. However, the loss in chemical energy was balanced by a reduction in the combustor skin friction. The optimum design determined from the parametric study was then used as the starting point for the optimization algorithm, which optimized the shape and length of the combustor/thrust surface for maximum thrust. The optimization algorithm manipulated Bezier control points that defined the bottom wall of the combustor/thrust surface to arrive at an optimum design that generated 19% more thrust than the initial design. The optimum shape of the thrust surface was similar to a classical bell nozzle shape.

The overall increase in thrust performance from the initial scramjet flow path design to the optimized flow path was not great enough to result in a design that would produce a net propulsive thrust for the scramjet engine concept studied. However, the increase in thrust performance through optimization was substantial since the total drag force for the initial design was 10.5 kN and the drag force for the optimized design was 4.2 kN. This 60% decrease in drag emphasises the benefits of using an optimization algorithm for scramjet design which seemingly only results in a small performance increases for the individual components of a scramjet engine.

The primary reason for the scramjet's poor thrust performance was the high wall shear stress or skin friction within the combustor, which resulted in a large drag force. A large percentage of the total skin friction drag was attributable to the skin friction within the combustor, which added to the drag at a rate of approximately 2.9 kN per square metre of combustor surface area. The combustor also contributed to the majority of the engine heating load at an approximate average heating rate of 3.6 MW per square metre of combustor surface area. The heat transfer rates were estimated by assuming that convective wall cooling with cryogenic fuel would provide an adequate cooling capacity for the engine to maintain the wall temperature at 1000 K. The high levels of skin friction and heat transfer that were calculated for the engine design in this study have shown that viscous boundary layer modelling is a very important issue that needs to be addressed when designing high Mach number scramjet engines. Under-estimating the skin friction may result in an engine design that does not provide a positive thrust.

The remainder of this section lists several recommendations for future scramjet research that are based on the results and discussion of this chapter.

(1) The high levels of calculated skin friction within the combustor suggest that an "internal" engine concept may be a preferred concept for axisymmetric scramjets to be flown at high Mach numbers. An internal engine would have a combustor with a small wetted surface area for a given flow area. This concept would also result in a decrease of the overall heat loading for the engine. A recent computational study of a scramjet inlet used an internal engine concept for these very reasons [240].

(2) The design study for the combustor/thrust surface in this chapter assumed that the hydrogen fuel was injected into the combustor flow perfectly mixed with the air. This simplification was used to minimize the computational time required for flow simulations. As a result of the simplification, the optimum scramjet combustor length was short since it needed only to be long enough for induction to occur and to get an adequate pressure increase in the bulk flow from the rapid combustion reaction. In reality, the combustor may need to be substantially longer to allow for adequate fuel mixing. Mixing can be slow for high flight speeds where the fuel needs to be injected close to parallel to the air-stream to provide momentum to the flow [27]. Therefore, the performance of the engine in terms of completeness of combustion may become mixing limited [63]. For this reason, it would be useful to investigate the effect that fuel mixing has on the optimal length and shape of combustors for high flight Mach number scramjets.

(3) The combustor for the scramjet designed in this chapter was essentially a constant area duct. For practical scramjet engines that may have a substantially longer combustor to allow for fuel mixing, the combustor may need to be made slightly divergent to allow for the growth of the boundary layer. As demonstrated in the parametric study of this chapter, the boundary layer growth in a long constant area combustor will tend to compress the combustor flow and increase the peak combustor temperature. As the peak combustor temperature increases, the Mach number of the flow decreases, and the amount of fuel that can be added to the flow before thermal choking occurs also decreases. This problem becomes worse as the flight Mach number decreases: "....very little heat can be added at low supersonic combustor entry Mach numbers (and correspondingly low supersonic flight speeds) in constant area combustors. Consequently, most practical scramjet engine designs utilise combustors incorporating area relief, either by step increases in area or by use of diverging duct segments" [48]. (p. 327). Other benefits that may be had by diverging the combustor are an increase in the extent to which the combustion reaction proceeds to completion, and a reduction in the combustor heat transfer.

(4) The scramjet design study presented in this chapter decoupled the design of the inlet and the combustor/thrust surface to make the design problem computationally practical. The shape of the cowl and combustor height were also constrained to simplify the design process. In future computational design studies, when computational resources increase, it is recommended that the scramjet engine be designed by modelling the entire flow-field with a single simulation so that the following design issues can be explored:

(i) The decoupled design of the scramjet inlet and combustor/thrust surface resulted in a

inlet that produced a shock-free flow into the combustor with minimal losses. However, there may be some advantage in having an inlet with high losses that produces a combustor entrance flow-field that interacts productively with the fuel, thus resulting in an overall increase in the engine efficiency over that obtained by an inlet with lower losses [177]. Also, there may be some advantage to having shocks and expansions entering the combustor since crossing shocks may generate local "hot spots" that can be used to initiate ignition. For a combustor could also be reduced, thus lowering the total combustor skin friction and heat transfer. However, there may be a problem with boundary layer separation induced by the reflected shocks within the combustor. Assessing the effect of shocks entering the combustor is a more realistic exercise since the no shock/expansion case (in the present study) will only occur at the on design condition.

(ii) The optimal inlet/combustor area-ratio was not explored in the current study since it was fixed to generate a specified combustor entry temperature [27]. The combustor entry temperature (and consequently the entry Mach number) can significantly affect the degree of dissociation at the combustor exit and the extent to which recombination occurs in the nozzle expansion [119].

(iii) The external cowl surface of the scramjet vehicle designed in this study was constrained and the optimum shape was not explored. There may be some benefit to having an external cowl surface that increases in radius towards the leeward end of the engine so that the expansion ratio of the thrust surface can be increased. The increase in thrust, may be greater than the extra drag incurred from the increased frontal area of the engine.

(5) In this study, boundary layer bleed slots in the walls of the engine were not examined because of the extra computational effort required to model the bleed flow path. The more simplified approach of using a bent cowl tip was used in preference to using boundary layer bleed slots prior to the combustor for reducing the possibility of boundary layer separation problems. However, boundary layer bleed slots may be the preferred method of avoiding boundary layer separation problems in an actual engine for a number of reasons: (i) Boundary layer bleed slots are more likely to be effective at off design conditions; (ii) By using boundary layer bleed slots, the entire external side of the cowl can be made parallel to the nominal flow direction, thereby reducing drag; (iii) Boundary layer bleed slots can be used for internal engine concepts, such as an engine with a funnel type inlet and a cylindrical combustor.

(6) Combustor skin friction and heat transfer were shown to be very high for the optimized design considered in this study. Two techniques that have been suggested to minimise the combustor skin friction and heat transfer are upstream port hole fuel injection and combustor wall injection (see Section 4.6). These ideas were not utilized in the present study, but they have the potential to improve the performance of high flight Mach number scramjets.

#### 4.7 Summary & Recommendations

(7) The air entering the scramjet engine in the present study was assumed to be composed of only  $N_2$ ,  $O_2$ , and Ar molecules, and all the chemical reactions involving these molecules were assumed to be frozen up until the combustor. This assumption was thought to be valid for determining the bulk fluid properties of the gas entering the combustor, however, the validity of the assumption for determining the correct ignition delay time was not determined. Small numbers of other molecules resulting from the dissociation of the air in the inlet, or trace molecules present in the free-stream, can significantly alter the ignition delay length. If the ignition delay length is longer than expected, then the combustion reaction will not proceed to the extent anticipated. Also, if the ignition delay length is shorter than expected, then the engine will incur extra skin friction from a combustor that is longer than required. Therefore, it would be wise to determine the sensitivity of the ignition delay length to the composition of the air entering the combustor in future studies.

(8) The combustor flow of the Mach 12 scramjet in this study was shown to be in vibrational non-equilibrium through an analysis of the slowest vibrational relaxation time for the gas mixture present in the combustor. However, the extent of the total internal energy of the gas flow that was in vibrational non-equilibrium was thought to be low. Primarily for reasons of time available to complete the current study, a vibrational non-equilibrium model was not added to the flow solver, so the entire combustor flow had to be assumed to be in vibrational equilibrium. A possible avenue for future research into computational optimization of high Mach number scramjets would be the implementation of a vibrational non-equilibrium model into the flow solver so that the effect of the simplification made in this study can be assessed.

(9) The design calculations for the scramjet engine relied on the accurate determination of skin friction at the walls of the scramjet. The turbulence model used to predict the behaviour of the boundary layers within the scramjet has a strong bearing on the accuracy of these skin friction estimates. The Baldwin & Lomax turbulence model, which has been extensively validated using low temperature skin friction and heat transfer experimental data was used in the present study. However, due to a lack of available skin friction and heat transfer experimental measurements, little is known of its (and for that matter any other turbulence model) accuracy for flow conditions such as those produced in high Mach number scramjet combustors. Therefore, experimental measurement studies in high enthalpy wind tunnels are required to confirm the predictive abilities of turbulence models if accurate design decisions are to be made using computational design tools.

# **Design of an Axisymmetric Shock Tunnel Nozzle**

As discussed in Section 1.2, part of the reason why the test flow quality of many high Mach number axisymmetric wind tunnel nozzles is poor, is due to the method used to design them. High Mach number nozzles designed with the classical method proposed by Prandtl & Buseman [11] in 1929, often show disturbances in the test flow. The disturbances arise because the design assumption that the boundary layer flow and core flow are uncoupled becomes inaccurate for high Mach number nozzles where the boundary layer makes up a large proportion of the exit flow area [25]. In this chapter, the design of an axisymmetric Mach 7 shock tunnel nozzle is discussed, where the method used to design the nozzle incorporates the design tool consisting of the PNS flow solver of Chapter 2 and the Nelder & Mead optimization algorithm discussed in Chapter 3. Unlike the method proposed by Prandtl & Buseman, this design tool takes into account the coupling between the boundary layer and the core flow.

The chapter starts with a description of a small reflected shock tunnel at The University of Queensland, where the flow processes that generate the test flow are discussed in some detail. The computational design method used for the design of the contoured, axisymmetric Mach 7 nozzle to be used in the small shock tunnel is then presented. The method consists of optimizing the expansion contour of the nozzle for minimal Mach number variation and flow angularity across the test core at the nozzle exit plane. The following sections discuss a grid refinement study and a sensitivity analysis of the flow quality produced by the optimized nozzle contour to the supply gas stagnation conditions. The chapter concludes with a brief summary and a recommendation for applying the design tool to nozzle design in the future.

### 5.1 The Small Shock Tunnel

The Small Shock Tunnel facility (locally known as the "Drummond Tunnel"<sup>1</sup>) at The University of Queensland, is a reflected shock tunnel with a fixed-length high pressure driver. It is primarily used for laser optics and the investigation of problems that are associated with larger reflected shock tunnels. Also, it is a relatively low enthalpy machine operating up to a maximum enthalpy of approximately 3 MJ/kg. Total temperatures in the nozzle supply region are limited to 2500 K so chemical and thermal non-equilibrium effects are minimal, making the analysis of test flows relatively simple.

The Small Shock Tunnel (SST) consists of a high pressure cylinder that contains the driver gas, a lower pressure cylinder (called the shock tube) that contains the test gas, a nozzle, a test section, and a dump tank (see Fig. 5.1). An aluminium diaphragm separates



Figure 5.1: Layout of the Small Shock Tunnel.

the driver and shock tube. This is the "primary" diaphragm and can be ruptured with the aid of a pneumatic piercing mechanism contained within the driver tube. The driver tube is typically filled with bottled high pressure helium or nitrogen to a maximum pressure of 6 MPa absolute; the shock tube is filled with test gas to a much lower pressure (on the order of 20kPa absolute). When the primary diaphragm ruptures, the high pressure driver gas expands into the shock tube and rapidly compresses the test gas via a shock wave. The primary shock, or incident shock, propagates along the length of the shock tube compressing and accelerating the test gas. The process is illustrated by a distance-time (x, t) wave diagram in Fig. 5.2.

The incident shock reflects off the nozzle contraction region where a cellophane or thin plastic secondary diaphragm is placed. The nominally stagnated high pressure and high temperature gas (or high enthalpy gas) generated by the reflected shock ruptures the

<sup>&</sup>lt;sup>1</sup>The name "Drummond Tunnel" is derived from the name of one of the investigators responsible for building the original tunnel [89].



Figure 5.2: Wave diagram of the shock and expansion processes that produces the test flow.

secondary diaphragm and then expands through the nozzle into the test section and dump tank, which are both evacuated to a low pressure prior to "firing" the tunnel. The test flow begins in the test section after the nozzle starting process has terminated and a steady expansion has been established. The nozzle starting process will be explored in more detail after first discussing the flow processes within the shock tube.

As the test gas drains through the nozzle, the reflected shock wave continues back up the shock tube and passes through the interface (or contact surface) between the driver gas and test gas. When the interaction of the shock and the interface produces no further shocks or expansion waves, the condition is said to be "tailored". This condition is characterized by a steady nozzle supply pressure and a contact surface that slowly moves towards the nozzle throat as the nozzle supply region drains (as illustrated in the top part of Fig. 5.2).

As the shock processes are occurring within the shock tube, the expansion waves emanating from the unsteady expansion in the driver section travel down the shock tube and nozzle and finally into the test section. The passage of these waves into the test section theoretically marks the end of the test time for tailored operation if the supply gas has not completely drained. In practice, the useful test time may have terminated well before these theoretical limits. Various studies have shown that complex interactions with the boundary layer of the shock tube and reflected shock can reduce the ideal test time [50, 206] through contamination of the test gas slug with driver gas. Bifurcation of the reflected shock into two oblique shock waves within the boundary layer can cause driver gas to "jet" along the wall and subsequently contaminate the nozzle supply region.

A typical unfiltered SST nozzle supply pressure history is shown in Fig. 5.3 for a tailored condition where helium is driving nitrogen. The condition was believed to be



**Figure 5.3:** Typical history of the nozzle supply pressure showing the principal events: (a) arrival of the incident shock; (b) reflected shock; (c) establishment of equilibrium pressure; (d) driver gas contamination (unfiltered shot 23069801).

tailored because it was initially derived from a time dependent numerical simulation of the facility where the contact surface was observed to be stationary, thus indicating a tailored condition [18]. When the test condition was experimentally established, the shock tube fill pressure was varied higher and lower than the numerically calculated fill pressure to assess if the condition was indeed tailored. The experimental results showed that the numerically calculated shock tube fill pressure gave the flattest time history of equilibrium pressure in the nozzle supply region which indicated a tailored condition.

The supply pressure transducer that produced the signal in Fig. 5.3 was positioned on the shock tube wall 68 mm upstream of the nozzle contraction (approximately one shock tube diameter). The time scale has been referenced to the passage of the initial shock which is well defined. Shortly after the initial shock passes the pressure transducer, the reflected shock passes in the opposite direction followed by a gradual increase in pressure to a maximum, then a slow decay. Close inspection of the increase in pressure due to the reflected shock shows that the pressure increase is stepped. This stepped increase in pressure suggests that the reflected shock is bifurcated into two oblique shock waves within the boundary layer containing a separation bubble. The gradual increase in pressure after the passage of the bifurcated reflected shock. This shock train would slowly decelerate the driver gas and cause the test gas pressure to increase. Eventually the drainage of the test gas through the nozzle causes the pressure to decay.



**Figure 5.4:** Quasi-one-dimensional representation of the nozzle starting process in both the physical and x-t plane [199]. Labelled features are: [a] primary shock; [b] contact surface; [c] upstream facing shock; [d] upstream head of unsteady expansion; [e] steady expansion.

The test gas drains through the nozzle throat and into the divergent part of the nozzle once the initial shock has reflected off the end of the shock tube and caused the light secondary diaphragm to rupture. The initial flow of the test gas through the nozzle forms a series of unsteady shocks and expansions as it moves down the nozzle. This process, known as nozzle starting, can significantly reduce the available test time for pulse facilities where the test time is of the same order as the nozzle starting time. A quantitative understanding of the starting process can be gained from the experimental and analytical studies of Amann [4] and Smith [199] and is briefly summarised in the following paragraph.

The rupture of the light secondary diaphragm causes a shock to form (labelled [a] in Fig. 5.4), which travels down the nozzle accelerating the low pressure gas already in the nozzle. Upstream of the shock is a contact surface (labelled [b]), which separates the test gas and the accelerated gas originally in the nozzle. The diverging walls of the nozzle slow the shock down, however, the test gas behind it is expanded to a high Mach number. This differential causes an upstream-facing shock (labelled [c]) to be formed which moves upstream relative to the mean fluid velocity, but has a net downstream motion due to the high fluid velocity. Between the upstream-facing shock and the steady expansion generated at the nozzle throat (labelled [e]), is an unsteady expansion ([c] to [d]), which also has a net motion downstream with velocity u - a. All of these waves eventually move out of the nozzle and into the test section after which time the test time begins. The time from the passage of the initial shock through the test section to the arrival of the steady expansion flow is largely a function of the nozzle geometry and Mach number

of the flow. Smith [199] noted that the starting time can be reduced for a given Mach number nozzle by increasing the nozzle expansion angle and reducing the size of the throat. Relatively large initial pressures in the nozzle prior to the arrival of the starting waves can also increase the nozzle starting time, however, this only becomes a concern for high stagnation temperature flows (> 3500K) [199, 74, 106].

The time required to establish a steady expansion within the nozzle is also governed by the attachment and stabilisation of the wall boundary layer. For long, high Mach number nozzles, the boundary layer on the nozzle is typically very thick and can take an appreciable amount of time to attach even after the starting waves have moved through the nozzle.

This discussion on the flow processes that produce the test flow for a reflected shock tunnel (such as the SST) provides a background for nozzle design, and highlights the important considerations that have to be made when designing a nozzle for a pulse facility that are not necessarily important for intermittent or continuous hypersonic flow test facilities.

## 5.2 Axisymmetric Mach 7 Nozzle Design

The design of a contoured, axisymmetric nozzle for the SST is used as both a demonstration and validation of the proposed design tool consisting of the *sm3d* flow solver and the Nelder-Mead optimization algorithm. The contoured axisymmetric nozzle was designed for a nominal exit flow Mach number of 7, and the expansion contour was optimized for a minimum Mach number and flow angle variation across the core flow at the nozzle exit plane. A nominal design Mach number of 7 was selected because a higher Mach number nozzle is not suited for the SST facility. The relatively low stagnation enthalpy of the SST test flow ( $\sim 2 \text{ MJ/kg}$ ) limits the maximum expansion ratio of the nozzle for useful test flow conditions that can be analysed with laser diagnostics and match real flight conditions. The boundary layers developed by a contoured Mach 7 nozzle were expected to be large enough to cause the assumptions in the MOC/BL nozzle design method to become inaccurate to such a degree that flow disturbances would be seen in the test flow if the nozzle had been designed with this method. The Mach 7 conical nozzle that was manufactured for the SST prior to the current study exhibits a boundary layer at the exit plane that occupies 60% of the total exit area [237]. It follows then that a contoured axisymmetric nozzle expanding to the same Mach number would have an equal or greater boundary layer thickness because of the extra nozzle wall length required to straighten the flow. Nozzles that develop boundary layers of this magnitude have been shown to produce only reasonable flow when designed with the MOC/BL technique [77, 114] due to the inaccurate representation of the characteristic reflection point [36]. On this basis,

then, a Mach 7 contoured nozzle for the SST facility could be considered a reasonable candidate for the demonstration of the new PNS/optimization based design tool.

The complete nozzle shape was broken up into three regions to simplify the design: (i) a subsonic contraction from the shock tunnel to the nozzle throat, (ii) an initial supersonic convex expansion that accelerates the flow from the nozzle throat to an inflection point, followed by (iii) a concave nozzle section that continues to expand and straighten the flow (see Fig. 3.3). Each section is joined continuously (that is, the second derivative is continuous) to minimise unwanted flow-field disturbances and difficulties in manufacture [197]. Continuity is achieved by defining each section with a Bézier curve. Bézier curves can be easily joined together continuously and are well suited to optimization (as discussed in Section 3.5).

### 5.2.1 Design Conditions and Constraints

The two design parameters that were fixed in the design of the nozzle were the throat diameter and the maximum wall expansion angle which typically occurs at the inflection point of contoured nozzles. The throat diameter was set at 7 millimetres to match the existing Mach 7 conical nozzle throat diameter. A throat of this size has been shown [237] to facilitate secondary diaphragm rupture using a light plastic diaphragm, and allows primary diaphragm particles (shrapnel) to pass through without getting jammed in the throat. However, small fragments of aluminium diaphragm of the order of a few millimetres are often seen in the dump tank of the facility. The drainage rate of the stagnated gas from the end of the shock tube is slow enough to maintain a reasonably constant nozzle supply pressure over the test time with a 7 millimetre throat.

The maximum expansion angle of the nozzle is strongly coupled to the nozzle starting characteristics and flow quality produced. As discussed in Section 5.1, starting processes are an important issue for hypersonic pulse facility nozzles because the starting time can be of the same order as the test time. By increasing the maximum divergence angle of the initial expansion, the nozzle length is reduced and the nozzle starting time is also reduced [199, 115]. However, as the angle is increased, a limit in the maximum expansion angle is reached where total wave cancellation by the concave wall contour is no longer possible. The theoretical angle limit is given by one-half the Prandtl-Meyer function [13] which is approximately equal to 45 degrees for Mach 7 flow. Theoretical wave cancellation is possible for this angle, however, in reality, a nozzle design with a 45 degree maximum expansion angle would produce poor test flow because of disturbances resulting from strong inviscid/viscous interactions. Propulsive rocket nozzles often use an expansion angle close to the Prandtl-Meyer limit to minimise the weight of the nozzle. The quality of the flow exiting from rocket nozzles is not a major design consideration since the

design objective is to maximise the thrust to weight ratio. Conversely, hypersonic test facility nozzles are generally designed with shallow expansion angles, much less than the Prandtl-Meyer limit, to minimise the flow-field disturbances [14]. However, too small an expansion angle will cause boundary layers to grow to impractical sizes over the increased nozzle length, and for pulse test facilities, the nozzle starting time becomes too great. Therefore, a balance must be reached to compromise the benefits at each end of the expansion angle range. Most axisymmetric hypersonic wind tunnel nozzles are designed with a maximum expansion angle between 10 to 15 degrees [199, 241, 197, 39, 115, 125]. Stalker believes that shock tunnel nozzles with expansion angles greater than 17 degrees will perform poorly because of possible problems with boundary layer separation (private communication with Stalker, R. J.). An inviscid expansion angle of 13.0 degrees was selected for the axisymmetric nozzle designed in this study.

The nominal nozzle supply conditions that the nozzle design was based on, were estimated from an established tunnel test condition used for the conical nozzle Pitot survey [18]. However, the actual nozzle supply conditions used for the experimental testing of the nozzle were significantly different (see Chapter 6). The reason for the difference in conditions was because of major upgrades that were made to the tunnel driver section and primary diaphragm station shortly after design work was started on the contoured axisymmetric nozzle. These changes had the effect of reducing the rupture pressure of the primary diaphragm and increasing the volume of driver gas. Consequently, the actual nozzle operating condition was not known at the time of the nozzle design. The established helium driver test condition for the SST prior to the modifications is shown in Table 5.1. The nozzle supply conditions and throat conditions listed in this table were calculated using measured shock speeds and numerical simulations. The details of these calculations are given in reference [18]. All the simulations were carried out assuming a calorically perfect gas.

The condition shown in Table 5.1 is significantly different to the test condition used for the nozzle survey which is shown later in Table 6.3. However, the quality of the flow in terms of the test core Pitot pressure profile at the exit plane of contoured nozzles for pulse facilities has been experimentally shown to be reasonably insensitive to nozzle supply conditions [114]. Therefore, the use of an imprecise design condition was not thought to significantly affect the quality of the final nozzle design. This hypothesis is computationally tested later in Section 5.4.

### 5.2.2 Subsonic Contraction

Stagnated gas at the end of the shock tube is accelerated to sonic throat conditions through the subsonic contraction. A smooth contraction profile from the end of the shock tube to

Test Condition				
Driver tube	Gas	Helium		
conditions	Fill pressure (MPa $\pm$ 0.05MPa)	4.0		
	Fill temperature (K $\pm$ 2K)	292		
Shock tube	Gas	Nitrogen		
conditions	Fill pressure (kPa $\pm$ 0.5kPa)	20.0		
	Fill temperature (K $\pm$ 2K)	292		
	Shock speed (m/s $\pm$ 40 m/s)	1188.0		
Nozzle supply	Pressure (MPa)	2.727		
conditions	Temperature (K)	2572		
(shock-compressed	Density (kg/m <sup>3</sup> )	3.57		
nitrogen)	Enthalpy (MJ/kg)	3.37		
Nozzle throat	Velocity (m/s)	872.5		
conditions	Density (kg/m <sup>3</sup> )	2.684		
(7mm throat)	Pressure (MPa)	1.456		
	Temperature (K)	1827		
	Mach number	1.001		
Dump tank gas	Air, pressure (Pa $\pm$ 20Pa)	400		
Primary diaphragm	Aluminium, thickness	0.6 mm		
Secondary diaphragm	Cellophane, thickness	0.01 mm		

 Table 5.1: Summary of the shock tunnel conditions prior to tunnel modifications.

the throat was used for the subsonic contraction and defined using a Bézier curve. Amann [4] states that subsonic contractions should be smooth in order to avoid separation and associated oblique shocks at the beginning of the initial expansion. Morel also suggests [155] that nozzle contractions should be designed with smooth continuous curves to avoid separation.

The contraction designed for the contoured axisymmetric nozzle is shown in Fig. 5.5. The contraction to a 7 millimetre throat from the shock tube diameter is performed over



Figure 5.5: Subsonic contraction design showing Bézier control points.

approximately 5 throat diameters and the wall contour has a maximum slope of 57 degrees

measured from the centre line. The Bézier control points were positioned to maintain surface continuity between mating parts.

### 5.2.3 Initial Expansion

The initial expansion expands the flow from the sonic throat to supersonic conditions using a divergent convex wall contour. The flow at the end of the initial expansion, often termed source flow, is straightened and expanded to the design Mach number by the concave expansion or turning contour. The shape of the initial expansion is somewhat arbitrary since the more critical process of flow straightening is performed in the concave section of the nozzle. However, a "gentle" expansion process should provide a more uniform diverging flow that can be more easily straightened. This section details the design process of the initial expansion for the axisymmetric Mach 7 nozzle. The inviscid contour of the expansion was determined first, then it was corrected for boundary layer growth. This design approach is somewhat inaccurate since it assumes that the core flow and the boundary layer flow are uncoupled. However, the errors made can be corrected in the subsequent design of the concave nozzle section where a coupled design method is used.

A four point Bézier curve was used to define the shape of a smooth continuous initial expansion from the nozzle throat as shown in Fig. 5.6. The curve was extended on



Figure 5.6: Initial expansion showing layout of Bézier control points.

the upstream end with a straight horizontal length equal to the throat diameter thereby creating an extended throat section. Zonars [241] stated that throats of this length produce "excellent high temperature source flow when measured in conical nozzles." A similar result is expected for contoured nozzles.

The Bézier control points p0, p1 and p2 were arbitrarily spaced 5 millimetres apart and the radial positions of points p0 and p1 were set equal to the throat radius to maintain curvature continuity. The radial position of control points p2 and p3 determine the maximum divergence angle at the end of the expansion which was set at 13 degrees for the inviscid design. The axial position of control point p3 and hence the overall length of the initial expansion was determined using characteristic tracing [15].

The characteristic tracing required a flow solution to be calculated for a guessed initial expansion design and the downstream region of the flow that is influenced by the initial

expansion. The space-marching flow solver, sm3d, was used to calculate an axisymmetric inviscid flow solution for an initial expansion design with a guessed overall length of 70 millimetres. The flow-field was extended a further 100 millimetres downstream by extending the wall with a straight line segment at 13 degrees as shown in Fig. 5.7. The



**Figure 5.7:** The boundaries of the computational domain used for the initial expansion characteristic tracing.

flow calculation used the throat conditions listed in Table 5.1 for the uniform conditions at the throat inflow plane. The throat gas velocity listed in the Table has a velocity slightly greater than Mach 1 to ensure that space marching flow calculations remain stable. The gas was assumed to behave as calorically perfect, diatomic nitrogen, and an unclustered grid of 4000 by 80 cells was used to discretized the computational domain. The simulation was run to a steady state and characteristic lines were traced through the solution. The characteristic that intersected the point on the nozzle centre line where Mach 7 flow existed was traced back to the wall. The point on the wall where the characteristic originated marked the length of the initial expansion. Figure 5.8 shows a plot of the Mach 7 characteristic intersects the wall at point A which set the initial expansion length at 48 millimetres. The section of the wall labelled A-B can only affect the shaded part of the flow-field. Therefore, the initial expansion 0-A completely specifies the non-shaded region x = 0 to x  $\approx 0.15m$ .

To complete the design of the initial expansion, an approximation of the boundary layer displacement thickness was added to the inviscid wall contour. The boundary layer displacement thickness was approximated by performing a viscous flow calculation for the inviscid expansion design using the turbulent boundary layer model of Baldwin & Lomax [20] with a compressibility factor in the damping coefficient (see Section 2.9). A turbulent boundary layer was assumed to develop from the nozzle throat rather than the nozzle supply region where the test gas starts moving. The turbulent boundary layer assumption was based on experimental comparisons with numerical simulations of the conical nozzle flow for the SST, which have shown that assuming the nozzle boundary layer to be turbulent gives accurate computational results [82, 18, 237]. The wall temperature of



**Figure 5.8:** Extended initial expansion showing (a) selected flow characteristics and (b) static pressure contours.

298 K since the flow is impulsive and it is unlikely that an adiabatic wall state would exist. The computational domain was discretized with a grid of 80 cells in the radial direction and 4000 cells in the axial direction where the radial cells were clustered towards the wall with an exponential clustering parameter of 1.01 (see Eq. 2.104). The safety factor used in Vigneron's coefficient (see Eq. 2.9) was set to 0.95 and the CFL number was set to 0.4 to maintain numerical stability. The convergence criteria for the flow calculation was set to a density residual of 0.01%.

Once the flow solution was obtained, the calculated velocity profile at the end of the expansion was integrated to using the relation,

$$\delta^* = \int_{\text{wall}}^{\infty} \frac{\rho}{\rho_{\infty}} \left( 1 - \frac{u}{u_{\infty}} \right) dr$$
(5.1)

to calculate the compressible displacement thickness of 0.26 millimetres. Adding this to the inviscid wall contour at the exit gives an expansion radius of 12.0 millimetres. The final coordinates of the Bézier control points for the initial expansion (as illustrated in Fig. 5.6) are given in Table 5.2 where the origin is taken to be at the start of the throat.

Two viscous, turbulent boundary layer flow solutions were computed for the initial expansion design using *sm3d*. High and low resolution simulations were performed using grids discretized with 80 and 40 cells respectively in the radial direction, and 10000 and 5000 cells respectively in the axial direction. The cells were radially clustered against the wall using an exponential clustering function (see Eq. 2.104) with a clustering parameter of 1.005. The radial clustering resulted in a  $y^+$  value of 2.7 for the cell closest to the

Control point	x, mm	r, mm
p0	7.0	3.50
p1	12.0	3.50
p2	17.0	4.68
p3	48.0	12.00

Table 5.2: Coordinates of the Bézier control points for the initial expansion.

wall at the exit plane in the low resolution case and 1.4 for the high resolution case. The cells were also clustered axially towards the throat with a clustering parameter of 1.5. The remaining details of the computational setup were the same as those for the flow calculation used to estimate the boundary layer displacement thickness. Figure 5.9 shows the computational mesh used for the low resolution computation and a plot of Mach number contours. The high and low resolution flow solutions at the exit plane of the initial



**Figure 5.9:** Parabolized Navier-Stokes simulation results for the nozzle initial expansion; (a) computational mesh; (b) Mach number contour plot (20 contours from 1.002 to 3.8)

expansion were used as the inflow conditions for the concave expansion flow calculations in the following sub-section.

Prior to the design of the concave flow straightening expansion, an estimate of the overall nozzle length was obtained from the inviscid flow solution of the initial expansion. The approximated length was obtained by extending a  $C_+$  characteristic from the intersection of the  $C_-$  characteristic and the axis at the Mach 7 location as shown in Fig. 5.10. The  $C_+$  characteristic was extended downstream in a straight line until it intersected the estimated edge of the boundary layer at the nozzle exit. The isentropic expansion ra-



**Figure 5.10:** Positive and negative flow characteristics intersecting the nozzle axis at the location where the Mach 7 test core begins.

tio for a Mach 7 inviscid flow is 104 which gives a exit radius of 35.7 millimetres for a 7 millimetre diameter throat. The exit radius was then increased to account for the turbulent boundary layer using the approximation [104]

$$\frac{\delta}{x}\sqrt{\mathrm{Re}_x} \approx 20 \tag{5.2}$$

which is derived from van Driest's compressible boundary layer approximations [236]. The Reynolds number was calculated as being  $5.1 \times 10^5$  using nozzle exit flow quantities calculated from isentropic relations. The Reynolds number length scale, x, was approximated as 400 millimetres. This gives a boundary layer thickness of 11.1 millimetres and, assuming  $\delta^*/\delta = 0.33$ , a displacement thickness of 3.7 millimetres. The edge of the boundary layer was then approximated as being at a radius of 28.3 millimetres. Extending the positive Mach 7 axial characteristic to this radius gives a nozzle length of 353 millimetres. To ensure that there is enough nozzle surface to straighten the flow, an extra 25 millimetres was added to this axial length giving an overall nozzle length of 378 millimetres.

#### 5.2.4 Concave Flow Straightening Expansion

The concave flow straightening expansion contour was designed by solving an optimization problem. The optimization problem consisted of a set of design variables that defined the concave expansion geometry and, an objective function defining the total variation of Mach number and flow angle for the core flow exiting the nozzle. The edge of the core flow was defined as the radial position where the axial velocity component was equal to 99% of the centre line velocity (approximate edge of the boundary layer). Using this independent definition of the core flow edge for each flow solution, lead to some difficulties that will be discussed later. Essentially, the optimizer was allowed to determine the absolute size of the core flow over which it would try to minimize the flow variation and on occasion, it would incorrectly attempt to achieve this goal by reducing the size of the core flow. The objective function for the optimization algorithm was defined so that the algorithm would attempt to find a nozzle shape that produced a flow with a minimum of variation in Mach number and flow angle across the core flow at the exit plane. All of the computational cells from the axis to the edge of the core flow at the exit plane were used to evaluate the objective function which was defined as,

$$Obj(dv) = (f_{\theta} + f_M)^2 \quad . \tag{5.3}$$

The two functions defining the variation in flow angle,  $\theta$ , and the distribution in Mach number, were

$$f_{\theta} = \frac{\phi_{\theta}^2}{N} \sum_{j=1}^{N} (v_j/u_j)^2$$

$$f_M = \frac{\phi_M^2}{N} \sum_{j=1}^{N} (M_{x,j} - M_{\text{design}})^2$$
(5.4)

where the symbol N denotes the number of cells in the core flow. Two weighting parameters,  $\phi_{\theta}$  and  $\phi_M$ , were used to scale the contributions of the flow angle variation function  $f_{\theta}$  and Mach number variation function  $f_M$ . The scaling parameters were set so that both functions would evaluate to 1 or less if all of the cells within the core flow have a variation in Mach number and flow angle less than a prescribed target. The optimization algorithm would then interpret both targets as equally important for achieving a satisfactory nozzle shape. The targets were set to a variation of Mach number across the core flow at the exit plane of less than 0.01 (or 0.14 %) and a variation of flow angularity less than 0.016 degrees (~ 1 arc minute). When or if the optimization algorithm found a design solution that achieved these targets, the optimization algorithm was stopped. These targets are "ideal" and were set very high to improve the convergence of the optimization search algorithm. Nozzle exit plane flow variations of this order can not be measured in pulse flow wind tunnels with the current generation of flow measurement instruments. The weighting parameters are equal to the inverse of the targets or design goals such that,

$$\phi_{\theta} = \frac{1}{\tan(0.016)} = 3.58 \times 10^{3}$$

$$\phi_{M} = \frac{1}{0.01} = 10^{2}$$
(5.5)

A Bézier curve was used to model the wall of the concave nozzle section where the difference in radial position between consecutive control points of the Bézier curve were used as optimization design variables. The Bézier curve was defined with seven control





Figure 5.11: Concave nozzle section showing Bézier control points used for optimization.

The axial positions of the remaining five control points (p0 to p4) were fixed in a distribution along the remaining length of the nozzle that was slightly clustered towards the nozzle throat. The overall axial length of the nozzle section was determined from the total nozzle length calculation discussed earlier in the previous section. The differences in radial distances between each pair of Bézier control points ( $p0_r - B_r$ ,  $p1_r - p0_r$ , ....) were used as design variables. This approach makes the design variables resemble wall slopes and improves the convergence of the design procedure [125].

The optimization of the wall contour was performed in two stages. First, a parametric study of the sensitivity of the optimization results to the initial wall contour designs was performed using a low resolution grid containing 40 radial cells. The best solution of the low resolution optimization study was then used as the initial solution for a high resolution optimization problem, which gave the final nozzle design. A set of eight optimization problems with different initial wall designs were used for the low resolution parametric study. Seven of the optimization problems used initial designs with smooth arcs to varying exit diameters and the eighth problem used an initial design with a conical expansion as shown in Fig. 5.12. The first seven initial designs were generated by locating the first



Figure 5.12: Initial nozzle wall contour designs for the low resolution optimization.

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upstream control point, p0, on a line extending from the first two fixed points, A & B (see Fig. 5.11), and the remaining control points were placed on a circular arc formed between p0 to p4. The radius of p4 was varied from 37.4 millimetres to 43.4 millimetres in 1 millimetre steps to give the seven designs (the estimated nozzle exit radius from Section 5.2.3 was 39.4 millimetres). The eighth design was generated by placing the design control points on a line from control point B to an exit radius of 37.4 millimetres. The initial perturbations of all the design variables were set to 2 millimetres except for the first upstream design variable perturbation which was set to 1 millimetre.

The computational grids for each of the low resolution optimization problems consisted of 40 cells in the cross-flow plane that were clustered towards the wall to maintain a  $y^+$  value for the cell closest to the wall equal to the  $y^+$  value at the exit plane of the low resolution initial expansion simulation which was 2.6. The algebraic turbulence model of Baldwin & Lomax [20] with a compressible damping term (see Section 2.9) was used to model the boundary layer growth along the nozzle wall and the gas was modelled as calorically perfect nitrogen. The inflow plane for each simulation was taken from the exit plane of the low resolution simulation for the initial expansion (see Fig. 5.9).

Each optimization problem was run on a single processor of a SGI Origin 2000 (see Appendix G) and took on average 5 hours for each of the eight cases (running at 66 seconds per flow solution). The optimization algorithm was terminated when the design goals were achieved or the variance of the simplex objective function values fell below 0.1 (see Eq. 3.1). The results of the eight low resolution optimization problems are summarised in Table 5.3. The results show that the sensitivity of the optimization algorithm to

Design	Starting exit	Initial	Converged	No. of objective
	radius, mm	objective value	objective value	evaluations
А	37.4	$12718 \times 10^{3}$	87.3	276
В	38.4	$6920 \times 10^{3}$	123.4	193
С	39.4	$3148 \times 10^{3}$	205.4	427
D	40.4	$1181 \times 10^{3}$	115.1	181
E	41.4	$300 \times 10^{3}$	104.5	329
F	42.4	$108 \times 10^{3}$	105.4	251
G	43.4	$124 \times 10^{3}$	147.0	207
Н	37.4	$10631 \times 10^{3}$	68073.2	319

Table 5.3: Results of the concave expansion optimization (H is the initial conical design).

the initial condition is low for well posed initial designs. However, case H shows that the performance of the optimization algorithm is poor for an initial design that is also poor (i.e. not similar in shape to the optimum shape). In optimization parlance, the algorithm is

susceptible to local minimum convergence. The optimized nozzle wall contours for each case are shown in Fig. 5.13. The first seven optimized designs are all very similar except



**Figure 5.13:** Optimized nozzle wall contours for the concave section. The solid lines depict the wall contours and the dashed line shows the variation in wall radius for the first seven cases.

for the end of the nozzle where the objective function becomes insensitive to the wall slope. The objective function becomes insensitive at the end of the nozzle because the domain of influence of the wall slope becomes limited to the boundary layer flow which is not considered in the objective function evaluation.

The nozzle expansion contour study used a simplex contraction coefficient of 0.5 as suggested by Nelder & Mead in their original paper [159] (see Section 3.2 for an explanation of the contraction coefficient). A 0.5 contraction coefficient was thought to give a good balance between rate of convergence and global minimum convergence. However, an inspection of the variation in final converged objective value for each of the design cases presented in Table 5.3 suggests that the local design space does not have a well defined global minimum and the contraction coefficient used may not be optimal. In an effort to improve the convergence of the optimization algorithm to the global minimum, the simplex contraction coefficient was increased to 0.75 which has the effect of slowing the contraction of the simplex. The parametric study with the eight initial design was then undertaken again using the increased contraction coefficient. The results of the eight optimization problems are shown in Table 5.4. The results show that increasing the contraction coefficient generally improves the ability of the optimization algorithm to converge to the global minimum for well posed problems (lower average converged objective function). However, the optimization algorithm, on average, required a greater number of objective function evaluations to converge to an optimal design. The optimized wall contours obtained using the increased contraction coefficient are shown in Fig. 5.14. The effect of the increased contraction coefficient is reflected in the reduced wall radius difference between all of the well posed design cases.

Increasing the contraction coefficient did not improve the optimization results for de-
Design	Starting exit	Initial	Converged	No. of objective
	radius, mm	objective value	objective value	evaluations
А	37.4	$12718 \times 10^{3}$	92.6	305
В	38.4	$6920 \times 10^{3}$	105.2	376
С	39.4	$3148 \times 10^{3}$	103.4	323
D	40.4	$1181 \times 10^{3}$	94.1	501
E	41.4	$300 \times 10^{3}$	103.9	312
F	42.4	$108 \times 10^{3}$	129.8	267
G	43.4	$124 \times 10^{3}$	108.8	517
Н	37.4	$10631 \times 10^{3}$	75077.3	437

**Table 5.4:** Results of concave expansion optimization with an optimization contraction coefficient of 0.75 (H is the initial conical design).



**Figure 5.14:** Optimized nozzle wall contours for the concave section using a contraction coefficient of 0.75. The solid lines depict the wall contours and the dashed line shows the variation in wall radius for the first seven cases.

sign case H with the conical initial design. The optimization algorithm converged to a design solution with an objective function of the same magnitude. In a second attempt to improve the optimization results for this poor initial design, the initial perturbations of the design variables were all increased to 10 millimetres. The larger initial perturbations give the simplex a greater initial range of exploration and give it a greater chance of converging to the global minimum. However, applying large perturbations to well posed initial designs may cause convergence to a local minimum that is found in the first few movements of the simplex (this hypothesis was not explored in the current study). A comparison of the optimization results for case H with the original 2 millimetre initial perturbation value and the 10 millimetre perturbation is shown in Table 5.5. Also shown are the results for a simplex contraction coefficient of 0.5 and 0.75 . In this case, the optimization results were substantially improved by increasing the size of the initial simplex, particularly for the 0.75 contraction coefficient case. The optimized wall contour designs are compared to the optimized design for case A in Fig. 5.15.

	Initial	Contraction	Converged	No. of objective
	perturbation, mm	coefficient	objective value	evaluations
	2	0.5	68073	319
	2	0.75	75077	437
	10	0.5	27426	378
	10	0.75	335	404
( r, m ( (	0.04 0.03 0.02 0.01 0.00 0.05 0.10	0.15 0.2	Case Case Case 20 0.25	A H, 0.5 contraction H, 0.75 contraction 

Table 5.5: Optimization results for case H with large initial perturbations of the design variables.

**Figure 5.15:** Optimized wall contours for case H with a large initial simplex size. Comparison is made with the optimized wall contour for case A with a 0.5 contraction coefficient.

Distance from diaphragm, m

The optimization design goals for the Mach 7 nozzle requires that the objective function evaluate to less than 2 for a satisfying design. However, the objective function evaluations for the best of the low resolution designs were approximately two orders of magnitude greater than the design goal required. An analysis of the optimized exit Mach number profile for the low resolution case A shows that the poor results are partly due to the definition of the core flow edge (or boundary layer edge). Figure 5.16 shows the exit Mach number profile for case A and the design goal tolerance for Mach number. Also shown on this figure are two definitions of the core flow edge. The core flow edge for the low resolution optimization cases was defined as the radial position where the axial velocity equalled 99.0% of the centre line velocity. This radial position is marked as  $0.99U_0$  in the figure. The objective function is evaluated using the Mach number distribution from the centre line of the nozzle to the edge of the core flow. For a core flow definition of  $0.99U_0$ , the optimization algorithm has tried to increase the Mach number towards the edge of the core flow in order to increase the Mach number of the cells just to the left edge of the core flow. These cells contribute to the large objective function value. If the core flow edge is defined as 99.9% of the centre line velocity (marked as  $0.999U_0$  in Fig. 5.16), the computational cells contributing to the high objective function value are significantly



**Figure 5.16:** Optimized exit plane Mach number for case A with a 0.5 contraction coefficient. The Mach number design goal is marked as well as the edge of the core flow using two edge definitions.

reduced.

The effect of changing the definition of the core flow edge was examined by repeating the case A optimization with the nominal contraction coefficient and the 99.9% core flow edge definition. A comparison of the optimized wall contours is shown in Fig. 5.17. The



**Figure 5.17:** Comparison of optimized wall contour for case A using two different definitions of the core flow edge.

optimization results were mixed in that the converged objective function evaluation for the 99.9% case was decreased to 16.0 (compared to 87.3 for the 99% case), but the wall slope at the exit of the nozzle became negative, thus compressing the flow at the exit. A nozzle with a negative wall slope is not a practical design solution and suggests that the objective function was not fully describing the desired objectives.

The exit plane profiles of Mach number and flow angle shown in Figs. 5.18 and 5.19 reveal why the objective function evaluated to a lower value. The 99.9% core flow



**Figure 5.18:** Profile of exit plane Mach number for case A optimization using two different definitions of the core flow edge.



**Figure 5.19:** Profile of exit plane flow angle for case A optimization using two different definitions of the core flow edge.

edge definition had the effect of reducing the region over which the objective function was evaluated. The reduction in the optimization region was caused by the relatively large initial perturbations of the initial design variables. The perturbations in wall slope caused perturbations in the exit plane flow velocity that were on the order of 0.1% of the centre line velocity. The edge of the core flow was then incorrectly identified and this caused the optimization algorithm to limit the region over which the objective function was evaluated. This region was reduced until the simplex became small enough through contractions to limit the large velocity perturbations.

Therefore, in order to prevent the optimization algorithm from reducing the core flow size while retaining the adaptive core flow estimation, it is necessary to match the core flow edge definition with the size of the initial perturbations that form the initial simplex. Using a 99.9% core flow edge definition requires that the initial design variable pertur-

#### 5.2 Axisymmetric Mach 7 Nozzle Design

bations be small. However, if small perturbations are used, and the initial design is not a good guess, the optimization algorithm is likely to converge to a poor local minimum. Therefore, it is prudent to use large initial design variable perturbations with a relaxed core flow edge definition to locate the design space containing the global minimum, and then use small perturbations with a stricter core flow edge definition to find the global minimum. This is the approach taken here where the low resolution case is used to find the approximate shape of the optimal nozzle design, and then the high resolution case is used to refine the shape to within the required design goals. Alternatively, a presumed core flow size could have been fixed, however, a conservative estimate would had to have been made prior to the calculation.

The optimized low resolution design solution for case A with the nominal contraction coefficient was used as the initial design for the high resolution optimization problem. The design variable perturbations that form the initial simplex were all reduced to 0.5millimetres, except for the first design variable closest to the nozzle throat which was reduced to 0.25 millimetres. The core flow edge was defined as 99.9% of the centre line velocity since the design variable perturbations were reduced, and the initial design was assumed to be close to the global minimum design. A computational grid of 80 cells in the cross-flow direction and 2000 cells in the axial direction was used to discretize the computational domain. The cells were adaptively clustered radially towards the wall to maintain a constant  $y^+$  value for the cells nearest the wall. The  $y^+$  value used was equal to the  $y^+$  value of the cell nearest the wall at the exit plane of the high resolution initial expansion calculation which was 1.4. The cells were also clustered axially towards the throat with an exponential clustering parameter of 1.1. The rest of the computational setup for the flow simulations was the same as the setup used for the low resolution simulations. The exit plane flow properties calculated for the high resolution initial expansion simulation were used as the inflow properties for the high resolution optimization. Only one optimization problem was solved with a simplex contraction coefficient of 0.5.

The optimization algorithm required 122 iterations to converge to a design solution with an objective function evaluation of 0.68, which took 21.2 hours to complete using one processor of the SGI Origin 2000. The variation in Mach number and flow angle at the exit plane of the optimized design solution are shown in Figs. 5.20 and 5.21 respectively (the physical edge of the nozzle at the exit plane is at a radius of 0.04196 m). The Mach number variation of the optimized design is within the design goal, however, the flow angle slightly exceeds the design goal in some regions of the core flow. An improvement in the flow angle variation may have been achieved by adding another Bézier control point and hence another design variable to the optimization problem. However, this was not carried out in the present study since the optimized design produces test flow that is very close to fulfilling the design goal, and the flow angle variation is below the precision



**Figure 5.20:** Mach number profile across the test core of the high resolution optimized nozzle design.



Figure 5.21: Flow angle profile across the test core of the high resolution optimized nozzle design.

of any pulse flow measurement instruments that are presently available.

A contour plot of Mach number is shown in Fig. 5.22 for the complete diverging nozzle design and the variation in centre line Mach number is shown in Fig. 5.23. The Mach number contours show that the length of the nozzle is approximately 40 millimetres longer than necessary. However, the current length maximises the test core volume since reducing the length will cause the expansion waves coming off the lip of the nozzle to cross the test core further upstream. The variation in axial Mach number is smooth and continuous and shows only a slight over-expansion at the start of the uniform flow region. Overall, the nozzle design is shown to expand the flow smoothly and to a highly uniform state at the exit plane. The computed variation in flow quantities at the exit plane of the nozzle are listed in Table 5.6 . Technical drawings of a Mach 7 nozzle that uses the nozzle contour designed in this chapter are presented in Appendix H.



Figure 5.22: Mach contours for the optimized Mach 7 nozzle.



Figure 5.23: Axial Mach number profile for the optimized Mach 7 nozzle.

## 5.3 Grid Refinement Study

A grid refinement study was undertaken for the optimized nozzle design to ensure that the solution produced by the computational scheme would converge to an exact solution if the grid resolution was increased. By "exact solution" it is meant the solution that would be generated by the flow solver using a computational domain disctretized with cells of infinitesimal size and by convergence, it is meant that the approximate solution to the PNS equations approaches the exact solution for the same initial boundary conditions as the computational grid is refined.

Four grids of increasing resolution were used to calculate nozzle flow solutions for the optimized nozzle design. The number of cells used in the radial and axial direction were doubled for every step increase in resolution. Each flow solution was obtained by first calculating the flow through the initial expansion then through the concave nozzle section. The calorically perfect throat conditions listed in Table 5.1 were used as the

	Average	$\pm$ Variation	
		Absolute	%
М	7.001	0.003	0.05
Angle, $^{\circ}$	-0.003	0.019	
Pressure, Pa	653.9	4.8	0.74
Temperature, K	202.4	0.2	0.09
Pitot Pressure, kPa	41.29	0.26	0.64

**Table 5.6:** Computed variation in flow quantities within the core flow at the exit plane of the optimized axisymmetric nozzle design.

uniform inflow conditions for each initial expansion calculation. The initial expansion grids were all clustered towards the wall using a clustering parameter of 1.005 (see Eq. 2.104) and the grids for the concave expansions were clustered to maintain the wall  $y^+$  value at the exit plane of the initial expansion (as was done for the design calculations). Each slice of cells was marched in time until the largest density residual decreased below 0.01%.

In order to assess whether the flow solutions were converging to a correct solution as the grid resolution was increased, the total axial force exerted on the nozzle was calculated and compared for each flow solution. The total axial force was calculated by integrating the surface pressure and viscous stress acting on the nozzle wall from the throat to the exit plane of the nozzle. The force acting on the nozzle is not a particularly relevant property for the current study, however, it was believed to be more sensitive to the flow solution than the objective function. Thus, comparing this value between grid resolutions would give a more accurate indication of the solution convergence.

Table 5.7 lists the number of radial and axial grid cells for the initial and concave expansion simulations, the concave expansion wall  $y^+$  values, and total calculated axial force acting on the nozzle from the throat to the exit plane for each of the flow calculations. The difference in calculated force between different grid resolutions can be used to determine the convergence order of the solution scheme as well as the estimated error. The solution scheme order of convergence, p, can be approximately determined using the relation,

$$p = \ln\left(\frac{f_1 - f_2}{f_2 - f_3}\right) / \ln(r)$$
(5.6)

where  $f_1$ ,  $f_2$  and  $f_3$  are the axial forces (or some other quantitative value) of the discrete solution for increasing grid resolutions, and r is the grid refinement ratio. Evaluating this expression using the axial force for the first three grids, gives a scheme order of 0.83 and

No. of radial	No. of	axial cells	Concave y <sup>+</sup>	Total nozzle
cells	Initial	Concave	wall value	axial force, N
20	2500	500	4.94	48.3
40	5000	1000	2.65	46.7
80	10000	2000	1.39	45.8
160	20000	4000	0.71	45.3

**Table 5.7:** Total calculated axial force exerted on the optimized nozzle design for grids of increasing resolution.

for the last three an order of 0.85. Since the calculated order is positive, it is fair to say that the solution converges as the grid resolution increases (up to the machine precision).

A generalised version of Richardson extrapolation [180] can be used to calculate an estimate of the fractional error in the quantity, f. The estimated fractional error, E, is given as

$$E_2 = \epsilon/(r^p - 1) \tag{5.7}$$

where

$$\epsilon = (f_1 - f_2)/f_2 \quad . \tag{5.8}$$

This error estimate is an ordered approximation to the actual fractional error of the quantity  $f_2$ . The approximated errors in calculated axial force for the three highest resolution grids were, 4.3 %, 2.5% and 1.4%. The consistently decreasing error also indicates a converging computational scheme. The error is plotted against the  $y^+$  value in Fig. 5.24 to show the trend of the decreasing error as  $y^+$  approaches 0.

#### **5.4** Sensitivity of Flow Quality to Stagnation Conditions

All the nozzle flow calculations up to this point were made using throat conditions that were calculated assuming a constant ratio of specific heats equal to 1.4. In reality, this assumption may be quite inaccurate. However, the design study was performed on the premise that the ability of the nozzle wall contour to cancel expansion waves and produce uniform exit flow was fairly insensitive to the gas ratio of specific heats [114]. This premise is tested here by performing a series of flow calculations over a range of enthalpies, using the final (optimized) nozzle shape and a more accurate gas thermodynamics model for calculating the nozzle throat conditions. The Mach number variation and flow angularity at the exit plane is then compared over the range of operating conditions.



Figure 5.24: Approximate solution error as a function of the wall  $y^+$  value for the computational cell nearest to the nozzle wall.

The investigation was begun by determining a range of throat conditions that are more realistic than the calorically perfect conditions listed in Table 5.1. Throat conditions were determined by first assessing the thermodynamic processes that were expected to be important as the gas flowed through the contraction and into the nozzle throat. The temperature of the gas in the nozzle supply region that flows into the nozzle throat is high enough to excite vibrational energy modes but not high enough to dissociate diatomic nitrogen. The excited vibrational energy modes are in equilibrium with the translational and rotational modes of energy in the nozzle supply region since the residence time of the flow in the nozzle supply region is large with respect to the vibrational relaxation time. As the flow is accelerated through the nozzle contraction into the throat, the residence time (or characteristic fluid time scale) becomes increasingly smaller and approaches the vibrational relaxation time of the nitrogen. The residence time of the flow in the nozzle throat can be estimated from the length of the nozzle throat (which is equivalent to the nozzle diameter in this case) and the flow speed through the throat. Also, the vibrational relaxation time for molecular nitrogen within the throat can be obtained from an empirical relation derived by Millikan & White [154] (see Eq. 4.1). The pressure, temperature and time scales of the gas within the nozzle throat are shown in Table 5.8 (these throat conditions were calculated using a calorically perfect gas model). The residence time is roughly an order of magnitude smaller than the vibrational relaxation time for nitrogen in the throat. This indicates that the equilibration of the vibrational energy mode with the other energy modes (translational/rotational) is occurring very slowly in comparison to the velocity of the gas (known as a thermodynamically frozen state). As the flow expands and accelerates downstream of the throat, the residence time reduces even further and the relaxation time increase as the gas cools. Therefore, the state of the gas in the expanding

p	$14.4 \mathrm{atm}$
T	$1827~{ m K}$
$\tau_{\rm residence}({\rm dia.}/u^*)$	$8.0 \mu s$
$ au_{\mathrm{vib}}(N_2)$	$81.1 \mu s$

 Table 5.8: Vibrational relaxation time and residence time for the nozzle throat.

section of the nozzle can be considered to be thermodynamically frozen. However, in the upstream section of the nozzle where the flow accelerates from the nozzle supply region through the nozzle contraction, it will undergo a transition from a thermodynamic equilibrium state, to a non-equilibrium state, then to a frozen state at the nozzle throat. This analysis indicates that the assumption of calorically perfect gas for the nozzle contraction flow calculations [18] is not accurate and the actual nozzle throat conditions may be significantly different from those used in the design of the Mach 7 nozzle (see Table 5.1).

To assess the sensitivity of the nozzle exit flow quality to the throat conditions, a series of flow calculations were performed using a range of throat conditions. The throat conditions were determined for five different stagnation enthalpies spanning  $\pm$  30% of the design stagnation enthalpy (2.67 MJ/kg). The throat density was fixed at 2.263 kg/m<sup>3</sup> for all the conditions and determined from isentropic relations (using  $\gamma = 1.4$ ) and the design stagnation density of 3.57 kg/m<sup>3</sup>. The gas sonic velocity and temperature at the throat were calculated using a thermodynamic equilibrium model [171] for nitrogen and an iterative process where the temperature of the gas was varied until it satisfied Eq. 5.9 for the given total specific enthalpy and density.

$$H_o = h(T) + \frac{1}{2}a(\rho, T)^2$$
(5.9)

The throat pressure and specific internal energy were also determined from the equilibrium model and are listed in Table 5.9 for the five total enthalpies being considered. This

$H_0/H_{0,\text{design}}$	$ ho^*$	$u^*$	$p^*$	$T^*$	$e^*$	$\gamma^*$
	kg/m <sup>3</sup>	m/s	MPa	Κ	MJ/kg	
0.70	2.263	760	0.9573	1425	1.1604	1.365
0.85	2.263	827	1.1408	1698	1.4241	1.354
1.00	2.263	888	1.3243	1971	1.6910	1.346
1.15	2.263	945	1.5055	2241	1.9596	1.339
1.30	2.263	997	1.6855	2508	2.2295	1.334

Table 5.9: Conditions used to test the sensitivity of the exit flow quality to operating conditions.

approach for calculating the throat conditions is still an approximation since the gas is assumed to be in thermodynamic equilibrium at all points in the nozzle contraction. As discussed previously, the gas is expected to be in thermodynamic non-equilibrium for a short duration in the contraction. Consequently, the actual ratio of specific heats would expected to be slightly lower than those listed in Table 5.9. However, the equilibrium assumption is an improvement over the calorically perfect assumption and, relevant to this discussion, the variation in specific heats is included.

The flow calculations downstream of the throat assumed the gas to be thermodynamically frozen where the ratio of specific heat was held constant at the throat equilibrium value. The flow states listed in Table 5.9 were used as uniform inflow conditions for each of the nozzle initial expansion flow calculations. Each of the five grids for the initial expansion had 80 cells in the radial direction that were clustered towards the wall with a clustering parameter of 1.005. The concave expansion grids were clustered towards the wall to maintain the wall  $y^+$  value at the exit plane of the initial expansion which ranged from 1.03 to 1.78. Figure 5.25 shows the exit plane Mach number profile for each of the five enthalpies. The average level of the exit Mach number is shown to decrease with the



**Figure 5.25:** Exit plane Mach number profiles for the optimized nozzle design with different flow enthalpies.

ratio of specific heats. This is consistent with the quasi-one-dimensional theory for a fixed area ratio isentropic expansion. The variation in exit plane Mach number is more clearly shown in Fig. 5.26 where the five Mach number distributions are plotted as deviations from their respective centre line Mach numbers. The variation in Mach number is within the design limits for most of the cases, however, the overall variation is not as small as the variation achieved when using a calorically perfect gas model. Figure 5.27 shows the calculated flow angularity at the exit plane of the nozzle for the five cases. All of the cases produce flow that is diverging in a uniform manner without any apparent disturbances. The amount of divergence decreases as the enthalpy decreases and the ratio of specific



**Figure 5.26:** Exit plane Mach number profile referenced by the centre line Mach number for the optimized nozzle design with different flow enthalpies.



**Figure 5.27:** Exit plane flow angularity for the optimized nozzle design with different flow enthalpies.

heats approaches 1.4. This trend in the exit flow is a result of the flow characteristics becoming steeper and not being correctly cancelled by the nozzle wall contour as the ratio of specific heats decreases.

The maximum deviation of the flow angle at the outer edge of the core flow for the highest enthalpy assessed was approximately  $0.5^{\circ}$ . To determine whether this deviation is measurable with experimental measurement techniques, the resulting variation in axial Pitot pressure downstream of the nozzle exit plane can be calculated. At a position 50 millimetres downstream of the nozzle exit plane, a  $0.5^{\circ}$  expansion in the nozzle exit flow would approximately correspond to a 3.4% reduction in the mean core flow Pitot pressure (calculated using a simple quasi-one-dimensional analysis and assuming  $\rho u^2$  approximately scales with Pitot pressure). This difference is within the current capabilities of Pitot pressure measurement in pulse flow wind tunnels (see Section 6.4). Therefore, in this case, the assumption that the quality of the nozzle flow is fairly insensitive to the gas

ratio of specific heats, is not acceptable for nozzles that are to be designed to achieve a flow uniformity that is greater than the resolution of current flow diagnostic equipment. This assumption may become even more inaccurate for the design of pulse flow wind tunnel nozzles where the tunnel supply gas (stagnation) enthalpies are much higher than those considered here.

The investigation of the flow quality sensitivity to the stagnation conditions in this section showed that the flow angle at the nozzle exit plane is sensitive to the gas ratio of specific heats. This result is contrary to the assumption made at the beginning of the chapter that the flow quality is insensitive to the gas ratio of specific heats. The insensitivity of the flow quality to the gas ratio of specific heats was suggested from the results of several Pitot pressure surveys for a nozzle designed using the MOC/BL method over a range of nozzle supply stagnation enthalpies [114]. The variation in the average Pitot pressure for these surveys was small, however, there were significant disturbances in the flow. If the flow had been more uniform, the variation in Pitot pressure for different stagnation enthalpies may have been apparent. Therefore, for the design of high quality nozzles to be used in high enthalpy pulse wind-tunnels, where a coupled design method is used such as the one described in this chapter, it would be prudent to employ a more accurate gas thermodynamics model than the calorically perfect model used in this chapter.

## 5.5 Summary & Recommendations

A Mach 7 axisymmetric shock tunnel nozzle contour was designed using a design tool consisting of a PNS flow solver and a Nelder & Mead gradient-search optimization algorithm, rather than using classical design methods. The design tool was used to optimize the concave expansion contour of the nozzle for minimal core flow Mach number variation and flow angularity. As part of the design process, an assessment of the optimization algorithm was made in terms of its ability to converge to the optimal contour shape for a initial contour shape that was considerably different to the optimal shape. The assessment showed that the algorithm was only capable of finding the optimal shape for such an initial shape by tuning its optimization parameters and increasing the initial step size. However, the optimization algorithm successfully converged to the optimal shape for a variety of initial shapes that consisted of simple smooth arcs. Therefore, it was not necessary to start with an initial contour designed using the MOC/BL technique as has been done in other studies [120].

The objective function used in the optimization of the nozzle contour was evaluated using only the Mach number and flow angle across the core flow at the exit plane of the nozzle. This approach contrasts with other approaches that also include a centre line Mach number distribution function as part of the objective function [125, 118]. As discussed in

#### 5.5 Summary & Recommendations

Section 3.5, a centre line Mach number objective function theoretically is not essential for effective nozzle optimization. The computational design study presented in this chapter showed that this was indeed the case, however, special care was required in defining the edge of the core flow to make the method work effectively. The edge of the core flow had to be defined so that the optimization algorithm did not try to reduce the size of the core flow region by over-expanding and re-compressing the flow. This was achieved by setting the definition of the core flow edge velocity to a value smaller than the lowest velocity produced in the core flow due to the initial simplex designs. This approach was applied successfully, however, two sets of optimization problems had to be solved to get the desired flow uniformity at the exit plane. The calculated flow-field of the final optimized nozzle contour was shown to have a test core flow angularity of  $\pm 0.02^{\circ}$ , a Mach number variation of  $\pm 0.05\%$  and a Pitot pressure variation of  $\pm 0.26\%$ .

A sensitivity analysis of the nozzle exit flow quality to the nozzle supply gas stagnation conditions showed that, for a given nozzle contour, the angle of flow divergence at the nozzle exit plane is a function of the gas ratio of specific heats. The analysis demonstrated that inaccurate modelling of the thermo-chemistry of the nozzle gas flow may lead to measurable deviations within the nozzle test flow. Therefore, an assumption of a calorically perfect gas state is not necessarily adequate for nozzle designs requiring high quality exit flow conditions, particularly for pulse facilities that run at high enthalpies.

The method used to design the axisymmetric nozzle in this chapter required the nozzle throat diameter and the maximum wall expansion angle to be specified as geometry constraints. These geometry constraints were used to define the shape of the convex section of the nozzle. To facilitate the design of the downstream convex nozzle section, the length of the nozzle was calculated using an approximation that was based on the MOC philosophy. Although this method was applied successfully in the current study, in hindsight, it was not the best way to approach the design problem.

A simpler way of designing the nozzle would have been to define the complete nozzle expansion contour with one Bézier curve, thereby including the initial expansion as part of the geometry to be optimized. The initial shape of the contour to be optimized could be determined by scaling an existing nozzle contour to the specified geometry constraints of a nozzle throat diameter and nozzle length. An approximate nozzle exit radius would also have to be specified to define the initial nozzle shape, however, this can be done with a simple inviscid calculation and an estimate of the boundary layer displacement thickness (as shown in this study, the convergence success of the optimization algorithm is reasonably insensitive to the initial nozzle exit radius if the initial shape of the nozzle contour is chosen wisely). The maximum wall expansion angle (which is predominantly a function of the specified nozzle length) would then be determined through the solution of the optimization problem. This approach for applying the design tool to the design of

nozzles would require a greater amount of computational time since the flow-field for the convex expansion is included in the design calculations. However, it is simpler than the method used in the current study and it would result in an optimum length for the nozzle shape. Also, the method could be easily reversed where the nozzle exit diameter and nozzle length are specified as geometry constraints, and the nozzle throat is determined by the design tool.

# Experimental Verification of an Axisymmetric Shock Tunnel Nozzle

This chapter is concerned with the construction, and Pitot pressure surveys, of the axisymmetric Mach 7 nozzle that was designed in Chapter 5 for the Small Shock Tube (SST) at The University of Queensland. The current chapter starts by presenting details of the nozzle manufacture and assembly, followed by a description of the instrumentation and data acquisition equipment that were used to perform the nozzle Pitot pressure survey. A new Helium driver flow condition used for testing the nozzle is discussed in the following section. Finally, the results of the Pitot pressure surveys are presented, which demonstrate the quality of the nozzle test flow and verify the method used to design the nozzle.

# 6.1 Nozzle Manufacture and Assembly

A sectional view of the assembled nozzle is shown in Fig. 6.1. The nozzle assembly was



**Figure 6.1:** Assembly of Mach 7 axisymmetric nozzle (O-rings and bolts have been removed for clarity).

manufactured in four separate parts: the nozzle contraction, initial expansion, concave expansion, and the throat shell that holds the nozzle together and locates it on the shock tube. A dump tank end cover was also manufactured to accept the new nozzle and provide a sliding seal. Detailed drawings for these components are included in Appendix H.

The nozzle assembly is fitted to the shock tube by rolling the dump tank back (left to right in Fig. 6.1) and then bolting the nozzle to the shock tube at the throat shell. Once fitted, the dump tank is then rolled forward until the end cover sits up against the shoulder of the nozzle. Access to the secondary diaphragm is achieved by sliding the contraction section out of the throat shell when the nozzle block is unbolted from the tube. All mating surfaces are sealed with O-rings.

The selection of the materials used for each component of the nozzle was based on the flow conditions through the component, the availability of the material, cost, and machineability. Table 6.1 lists the materials used. The throat shell and end cover were

Item	Material
Contraction	316 Stainless steel
Initial expansion	316 Stainless steel
Concave expansion	2011 T6 Aluminium
Throat shell	316 Stainless steel
Dump tank end cover	C-Mn Steel, plated with 5 microns of chrome

Table 6.1: Materials used to manufacture nozzle block and end cover.

manually machined using a conventional lathe as were the exteriors of the other components. A numerically controlled (NC) lathe was used to machine all the contoured surfaces. The maximum axial travel of the NC lathe cutting tool was fixed at 340 millimetres and the maximum cutting diameter was 500 millimetres. An AT clone computer running POLARIS was used to down-load the cutting tool path into the lathes internal memory which was limited to 700 points. Each component was machined separately so 700 points could be used to define each contour. This limit was acceptable for the short nozzle contraction and initial expansion sections, however, the 330 millimetre concave expansion had a perceptible "waviness" in the final cut surface since the distance between each cutting point was 0.47 millimetres. The "waviness" was removed with hand finishing using a fine grade abrasive paper.

Another flaw that occurred in the manufacture of the nozzle was an unwanted flare on the up-stream lip of the concave expansion. The flare resulted from the force applied to the acute corner by the NC cutting tool. This flaw was removed by facing off the upstream mating surface of the concave expansion and then backing it with some scrap which supported the corner in the machining process. The nozzle contour was then displaced 1 millimetre upstream to cut out the flare, thereby reducing the length of the throat by 1 millimetre.

After the components were machined, a maximum difference in the diameter of  $\pm 0.08$  millimetres was measured at the connection between the initial expansion and the concave expansion. This error was thought to be due to the deflection of the 400 millimetre cutter support. Micol [150] makes the point that disturbances in nozzle test flows can be a result of misalignment between nozzle sections and suggests a tolerance of  $\pm 0.025$  millimetres which is less than a third of the tolerance achieved in the manufacturing of the current nozzle.

When the nozzle was assembled, fitted to the shock tube and tested for leaks under a vacuum, a leak was identified at the union between the shock tube and the throat section, which was the result of a design flaw. The nozzle contraction was designed slightly longer than was required to provide a clamping force when engaged with the shock tunnel spigot (see Fig. 6.2). This force ensured the internal O-rings sealed effectively. However, the



Figure 6.2: Design flaw in nozzle contraction.

extra length separated the throat shell and shock tube to a point where the O-ring that seals this section became ineffective. The flaw could not be completely removed from the nozzle because the design has too many critical dimensions. Different secondary diaphragms will have different thicknesses and hold the throat shell at varying distances away from the shock tube. However, the design was corrected for the thickness of the diaphragm used in the Pitot survey by machining 0.5 millimetres off the length of the contraction. The nozzle block was well sealed after this modification.

# 6.2 Instrumentation and data acquisition

The SST is equipped with a Pitot rake mounted on a horizontal sting that is attached to the back of the dump tank. The Pitot rake can accommodate four Pitot probes spaced 28

millimetres apart, however, only three Pitot probes were required for the nozzle survey (see Fig. 6.3). Each Pitot probe contained a PCB piezoelectric pressure transducer (model No. 112A21) mounted behind a small perforated brass shielding disk to protect it from diaphragm shrapnel (see Fig. 6.4). Technical specifications for the PCB transducers are presented in Appendix I. The leads from the pressure transducers were connected to



Figure 6.3: Pitot rake positioned 1 millimetre from the exit plane of the nozzle.



Figure 6.4: Sectional view of a Pitot probe used in the nozzle survey.

a constant current power supply and then to a 4 channel digital oscilloscope (Yokogawa model 7006 DL12000A) for signal recording. The start of signal recording was triggered off the incident shock signal from the nozzle supply piezoelectric pressure transducer mounted on the shock tube wall (see location B in Fig. 6.6). A second oscilloscope was used to record the signal from the wall mounted heat transfer gauge.

Data signals were recorded at a sampling rate of 2 MHz with 10,000 8-bit samples being recorded for each channel over a 5 millisecond interval. The signals recorded

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#### 6.2 Instrumentation and data acquisition

by the oscilloscope were transfered to a 486 IBM-compatible computer for storage and data analysis via a General Purpose Interface Bus (GPIB) card (National Instruments AT GPIB/TNT). A LabView script was used to capture the data, display it and save it to disk. The saved data was then processed with a C program that filtered and averaged selected data over a nominal test time range.

Prior to performing the nozzle Pitot survey, a calibration of the pressure transducers was performed with the pressure transducers mounted within the Pitot probes in the rake as they were during the Pitot survey (see Fig. 6.5). The transducers were calibrated using a small gas cylinder that was filled with nitrogen to a known pressure. The cylinder was fitted with a calibrated pressure gauge and an electronic solenoid valve. Extending from the exit port of the solenoid valve and into the dump tank, was a length of brass tube with an O-ring sealing arrangement in a recess at the end. The whole apparatus was moved up to each Pitot probe in turn and the brass tube was sealed against the end of the probe. The pressurised nitrogen gas was then released from the gas cylinder by actuating the solenoid valve. The resulting signal from the pressure transducer was recorded on the digital oscilloscope.



Figure 6.5: Pressure transducer calibration arrangement.

Each transducer was tested at five different pressure levels and three shots were performed at each pressure. Plots of voltage against time for each of the three Pitot transducers are included in Appendix I, together with the data reduced plots of pressure against measured voltage. The calibration chart for the pressure gauge fitted to the cylinder is also included in Appendix I. Lines of best fit were placed through the plots of pressure versus voltage to determine the transducer sensitivities listed in Table 6.2. Also shown in the table are the nominal manufacturer sensitivities which are significantly different. A possible reason for the difference may be that the gauges are sensitive to the mounting arrangement. The stagnation pressure transducer was calibrated in earlier experimental work [18] and the results are also listed in the table.

Gauge	Model	Serial	Sensitivity, k	Pa/V
Location	Number	Number	Manufacturer's	Present
Pitot 1	112A21	14534	136.9	146.0
Pitot 2	112A21	14535	138.8	147.1
Pitot 3	112A21	14536	132.2	135.1
Stagnation	111A26	7450	689.5	688.4

 Table 6.2: Pressure transducer sensitivities.

## 6.3 Test condition

Shortly after the nozzle design was completed, the small shock tunnel (SST) was upgraded by making the driver longer and modifying the diaphragm station to allow for a cleaner primary diaphragm rupture with a piercing rod [46]. During the manufacture of the nozzle, a new test condition was established for the upgraded facility using the Mach 7 conical nozzle. The new rupture pressure for the 0.6 millimetre aluminium primary diaphragm was found to be 3.30 MPa (gauge) by simply filling the driver with a known gas pressure until the diaphragm burst. The test condition driver fill pressure was then set slightly lower at 3.25 MPa (gauge) so that the piercer could be used to initiate the shot. An estimation of the shock tube fill pressure for a 3.25 MPa Helium driver was obtained by scaling the shock tube fill pressure for the 4 MPa Helium driver test condition that was used prior to the facility modifications [18]. The final shock tube fill pressure was obtained by performing several trial shots, where the pressure was iteratively varied higher and lower than the scaled pressure to find the optimum tailored condition. The new condition was established with a Helium fill pressure of 3.25 MPa (gauge) in the driver section of the tunnel and a Nitrogen fill pressure of 16.5 kPa (absolute) in the shock tube (see Table 6.3).

To characterise this new condition, the nozzle supply pressure and shock speed were recorded over several shots. The shock speed and nozzle supply pressure were measured with the heat transfer gauge and the PCB piezoelectric pressure transducer that are mounted on the wall of the shock tube. The heat transfer gauge is mounted on the tube wall 217 millimetres upstream of the pressure transducer which itself is mounted a 68 millimetres upstream of the nozzle contraction (see Fig. 6.6). The measured time between the arrival of the incident shock between the two transducers was used to calculate the shock speed. The nozzle supply pressure was approximated by the pressure signal from the piezoelectric pressure transducer.



**Figure 6.6:** Schema of the Small Shock Tunnel facility fitted with the contoured Mach 7 nozzle showing principle dimensions in millimetres. A wall mounted heat transfer gauge is mounted at A and a PCB pressure transducer is mounted at B. The pneumatic cylinder and piercer occupy a volume of approximately 530cc.

Predictions of the quasi-steady gas conditions within the nozzle supply region and nozzle throat were determined from the results of a one-dimensional simulation of the shock tube facility. A Lagrangian CFD code (L1D) [103] was used to perform the simulation which has been shown to simulate the gas dynamics of shock tunnels with reasonably accuracy [108, 113]. The computational domain of the simulation was based on the dimensions of the shock tube facility shown in Fig. 6.6. The gas states of the computational cells that modelled the driver and shock tube were initially set to the fill conditions listed in Table 6.3. The cells for the nozzle and test section were set to a condition of room temperature air at an absolute pressure of 400 Pa (3 torr). The nitrogen test gas was thermodynamically modelled with a vibrational equilibrium model [171], and the helium driver was modelled with a calorically perfect model as was the low pressure air initially in the nozzle and test section. The time accurate simulation was initiated at the rupture of the primary diaphragm and was terminated 4 milliseconds after the rupture. The simulation, containing 1020 cells, was performed on one processor of a SGI Origin 2000 (see Appendix G) and took 4 hours 38 minutes to complete.

The measured pressure from the nozzle supply pressure transducer was compared with the calculated pressure at the transducer location to assess the accuracy of the simulation. The two pressure traces are shown in Fig. 6.7. Good agreement is shown between the two traces, except for the region just after the reflected shock where the experimental trace does not reach the same post shock pressure as the simulation. This is a result of the complex shock-reflection process not fully modelled in the calculation [50, 206]. The speed of the incident shock travelling down the shock tube was extracted from the simulation data and compared with the experimental shock speed (listed in Table 6.3). The two speeds differed by only 2.2% (30 m/s) which is less than the experimental measurement error of 2.9%.



**Figure 6.7:** Static pressure traces at a point 68 millimetres upstream of the nozzle contraction. The solid line represents the experimental trace and the dashed line is the calculated pressure (shot No. 23069801 filtered).

For a short period of time following shock reflection, it is assumed that the gas conditions in the nozzle-supply region are steady, and that, as far as experimental measurements are concerned, the processing of the shock-heated gas occurs as a steady expansion through the converging-diverging nozzle. The quasi-steady nozzle supply conditions were approximated as being the simulated conditions at the nozzle supply pressure transducer location at a time of t = 0.84 milliseconds in Fig. 6.7. The calculated nozzle supply condition at this time is given in Table 6.3. The nozzle throat condition was then calculated by first determining the ratio of specific heats for the supply condition and then computing the isentropic throat density as,

$$\rho_* \simeq \rho_o \left(\frac{2}{\gamma_o + 1}\right)^{\frac{1}{\gamma_o - 1}} \quad . \tag{6.1}$$

The throat density and total enthalpy were then used in Eq. 5.9 with a vibrational equilibrium model [171] to iteratively solve for the throat temperature and the other flow properties as listed in Table 6.3. Finally, the test section condition was obtained from a PNS simulation of the optimized nozzle design using the approximated throat conditions as uniform inflow conditions. The computational grid and solver configuration described in Section 5.4 was used for this simulation, and the nitrogen gas was assumed to be thermodynamically frozen downstream of the throat with a ratio of specific heats equal to 1.355. The flow quantities listed are the average values within the core flow at the nozzle exit plane.

Test Condition				
Driver tube	Gas	Helium		
	Fill pressure (MPa $\pm$ 0.05MPa)	3.25		
	Fill temperature (K $\pm$ 2K)	292		
Shock tube	Gas	Nitrogen		
	Fill pressure (kPa $\pm$ 0.5kPa)	16.5		
	Fill temperature (K $\pm$ 2K)	272		
	Shock speed (m/s $\pm$ 40 m/s)	1370		
Nozzle supply	Pressure (MPa)	2.304		
	Temperature (K)	1932		
	Density (kg/m <sup>3</sup> )	4.02		
	Enthalpy (MJ/kg)	2.23		
Nozzle throat	Velocity (m/s)	819		
	Density (kg/m <sup>3</sup> )	2.53		
	Pressure (MPa)	1.254		
	Temperature (K)	1668		
Test section	Velocity (m/s)	1979		
	Density (kg/m <sup>3</sup> )	0.0094		
	Pressure (Pa)	586		
	Temperature (K)	210		
	Mach number	6.8		

**Table 6.3:** Summary of the shock tunnel conditions used for nozzle calibration (all pressures are absolute except for the driver tube which is a gauge pressure).

### 6.4 Results of Pitot Pressure Survey

The test flow quality of the manufactured nozzle was assessed by conducting two Pitot pressure surveys of the flow issuing from the nozzle. One survey was performed 1 millimetre downstream of the nozzle exit plane, and a second at a plane 58.5 millimetres downstream. The purpose of the second downstream survey was to determine the amount of divergence in the core flow.

The first survey had the rake positioned with the upstream ends of Pitot probes 1 millimetre downstream of the nozzle exit plane. A complete survey across the exit flow of the nozzle was compiled from an ensemble of 11 shots, where the rake was moved in the cross-stream direction in increments of 3 millimetres between shots. A typical Pitot pressure transducer signal and supply pressure signal are shown in Fig. 6.8, where time t = 0.0 represents the passage of the initial shock past the wall mounted supply pressure transducer in the shock tube. The supply and Pitot pressure signals shown in this figure were filtered using a moving average filter with a half-width of 10 data points (or 5  $\mu$ sec half-width).



**Figure 6.8:** Wall pressure history in the nozzle supply region and Pitot pressure history at the 1 millimetre nozzle exit plane (shot 24069804 filtered).

The discrete Pitot pressure values presented in the Pitot survey plots, were obtained by averaging each Pitot pressure signal over a test period from time t = 0.8 ms to t =1.4 ms (see Fig. 6.8). The nozzle starting waves had clearly passed through the test exit plane by t = 0.8 ms and the pressure level is seen to slightly decrease after time t = 1.4ms. The upstream Pitot survey is shown in Fig. 6.9, where the bars indicate the standard deviation of the unfiltered pressure signal during the test period. Shown also are the Pitot pressure values normalized by the average nozzle supply pressure over the same length of time, but 0.25 milliseconds earlier. The radial positions where there are two data points indicates that a repeat shot was made in this position with the PCB pressure transducers swapped around in the rake. The average Pitot pressure across a core flow region of  $\pm 25$ millimetres is 33.5 kPa with a standard deviation of  $\pm 1.6\%$ . The Pitot pressure signals showed a large amount of noise as indicated by the bars in Fig. 6.9. The average of the standard deviation of noise in the core flow region was  $\pm$  10.4% of the measured Pitot pressure. This noise level is far greater than the standard deviation in average Pitot pressure across the core flow which was  $\pm 1.6\%$ . Despite the quality of the signals, it is clear that there are no large disturbances in the core flow and the flow is reasonably symmetrical about the centre-line of the nozzle.

A large part of the variation in Pitot pressure during the test time appeared to be caused by oscillations at a distinct frequency. The dominant frequency seen in the majority of the Pitot traces was  $\sim 31$  kHz. A similar result occurred in earlier nozzle calibrations of the Mach 7 conical nozzle [237] where the dominant frequency of the noise was ap-



**Figure 6.9:** (a) Measured Pitot pressures and (b) normalized Pitot pressures across the exit plane of the nozzle 1mm downstream. Bars indicate the standard deviation of the unfiltered pressure signal during the sampling time.

proximately 37 kHz. The same Pitot rake was used in the conical nozzle survey with different PCB pressure transducers of the same model. One possible explanation for the noise could be aerodynamic resonance. Each Pitot probe has a forward facing cavity that may resonate due to small disturbances in the flow thus amplifying the disturbance [60]. It is expected that the free-stream flow is smoother than indicated by this experimental data.

The second Pitot survey was performed at a location 58.5 millimetres downstream of the nozzle exit plane. The measurement and analysis procedure used for the upstream survey was also used for the downstream survey. The resulting Pitot profile for the downstream survey is shown in Fig. 6.10. A prominent feature of the Pitot pressure profile are the peaks occurring at the edge of the core flow. An analysis of the Pitot pressure signal traces revealed that these peaks are only present in the flow over a limited time period not long after flow starting. The time period is shown on the filtered signal traces were also observed for all the Pitot pressure signals within the peak regions. The peaks appear approximately 0.95 milliseconds after the passage of the initial shock and then dissipate by 1.4 milliseconds. Since the sampled time period for the Pitot survey (0.8 to 1.4 msec) contains this entire time period, the peaks are quite visible in the Pitot surveys. The reason



**Figure 6.10:** (a) Measured Pitot pressures and (b) normalized Pitot pressures across the exit plane of the nozzle 58.5mm downstream. Bars indicate the standard deviation of the unfiltered pressure signal during the sampling time.



**Figure 6.11:** Pitot trace of probe at the centre of the left peak. The time that the peak remains a dominant feature of the survey is marked by the dashed lines (shot 07079801 filtered).

for their existence was thought to be due to unsteady test section wave interaction caused by the relatively high static pressure within the test section and dump tank prior to the shot (400 Pa or 3 torr)<sup>1</sup>.

In order to investigate this theory, a transient, axisymmetric flow calculation of the nozzle starting process and test flow development was performed using a time-dependent Navier-Stokes flow integrator [110] (calculation performed by P.A. Jacobs). The simula-

<sup>&</sup>lt;sup>1</sup>Typical test section and dump tank pressures used for the larger T4 reflected shock tunnel at The University of Queensland are approximately 0.5 torr.

Mach 7 nozzle.

tion domain included a downstream section of the shock-tube, the nozzle, and the testsection. The inflow condition at the upstream plane of the modelled shock tube section was the estimated flow condition behind the incident shock. Turbulent boundary layer growth was modelled along the walls using the Baldwin & Lomax algebraic eddy viscosity model [20], and the gas was assumed to behave as calorically perfect nitrogen and air. The initial quiescent gas states within the shock tube and nozzle/test-section were the same as the gas states used in the actual flow experiments and are shown in Table 6.4. The temperature contours for the flow solutions at times 0.8, 1.1, 1.2 and 1.5 milliseconds

 $Gas \quad \rho \text{ (kg/m^3)} \quad u \text{ (m/s)} \quad p \text{ (kPa)} \quad T \text{ (K)}$ 

Table 6.4: Initial gas conditions used in the time accurate simulation of the SST with the contoured

	Gas	ho (kg/m <sup>3</sup> )	<i>u</i> (m/s)	p (kPa)	T (K)
Post shock	$N_2$	0.8621	1130.0	320.1	1250
Shock tube	$N_2$	0.1865	0.0	16.5	298
Nozzle/test-section	Air	0.0047	0.0	0.4	298

after the passage of the initial shock past the location of the wall mounted supply pressure transducer in the shock tube (location B in Fig. 6.6) are shown in Fig. 6.12. The 0.8 and 1.5 millisecond flow solutions show the structure of the flow before and after the peaks in the downstream Pitot profile occur, and the 1.1 and 1.2 millisecond flow solutions show the structure of the flow during the occurrence of the peaks. The converging waves across the downstream area of the test flow in the 1.1 and 1.2 millisecond frames were thought to result in the peaks seen in the downstream Pitot pressure profile. The wave structure around the free jet issuing from the nozzle seems to cause these converging waves. By reducing the quiescent static pressure within the test section and nozzle prior to the shot, the effects of this wave structure may be reduced. However, this idea is speculative and needs to be confirmed with further flow experiments and transient flow calculations, which were not performed in the course of this study.

The idea of reducing the initial static pressure to eliminate the downstream test flow disturbances is supported by the results of a Pitot pressure survey for the 20 Inch, Mach 6,  $CF_4$  Tunnel at the NASA Langley Hypersonic Facilities Complex [152]. The 20 Inch Mach 6 tunnel is a lead-bath-heated, intermittent blow-down facility, fitted with a contoured, axisymmetric Mach 6 nozzle. The maximum run time for the tunnel is 30 seconds. The survey results reported by Miller [152] show the Pitot pressure profile in the cross-stream direction at a location 6 inches (or 152 millimetres) downstream of the nozzle exit plane. Two profiles are shown for the Pitot pressure at this location. One is for a time of 6 seconds after the initiation of the test flow, and the other is for a time of 11 seconds after the initiation of the test flow. The profile at 6 seconds is clean and uniform, however, at



**Figure 6.12:** Temperature contours from a time-accurate simulation of the Small Shock Tube fitted with the axisymmetric, contoured Mach 7 nozzle. Time, t, is the approximate time in milliseconds after the passage of the initial shock past the supply pressure transducer (calculation by P. A. Jacobs).

11 seconds, two spikes appear in the profile at the outer edges of the core flow. The 11 second profile is very similar to the profile shown in Fig. 6.10. The spikes in the 20 Inch Mach 6 tunnel exit flow were attributable to the increasing pressure within the test section over time.

Despite the peaks in the downstream nozzle Pitot profile, the average Pitot pressure in the core flow could still be compared with the upstream value to get some idea of the amount of flow convergence/divergence. The average downstream Pitot pressure within a  $\pm 20$  millimetre test core was 34.4 kPa with a standard deviation of  $\pm 2\%$ . The downstream average is 2.7% higher than the upstream average, which suggests that the flow is converging. An estimate of the flow convergence angle at the outer edge of the core flow can be obtained by a simple quasi-one-dimensional analysis, where the flow is assumed to undergo a conical compression from the nozzle exit plane. From this analysis, the maximum flow angle for the core flow at the exit plane of the nozzle was estimated as being  $0.35^{\circ}$  towards the nozzle centre line.

A comparison of the experimental Pitot pressure survey results at the nozzle exit plane was made with the nozzle exit plane Pitot pressure estimated by the computational results of Section 6.3. The computational Pitot pressure was calculated using the "Rayleigh Pitot tube formula" [10] and the calculated exit plane velocity and density. The formula is shown in Eq. 6.2 and equates to  $0.92\rho u^2$  for a Mach number of 6.5 and  $\gamma$  of 1.355.

$$p_{\text{pitot}} = \rho u^2 \left\{ \left[ \frac{(\gamma+1)^2 M_{\infty}^2}{4\gamma M_{\infty}^2 - 2(\gamma-1)} \right]^{\frac{\gamma}{\gamma-1}} \left[ \frac{1-\gamma+2\gamma M_{\infty}^2}{\gamma+1} \right] - 1 \right\}$$
(6.2)

The computational and measured Pitot pressure at the exit plane of the nozzle is shown in Fig. 6.13. Also shown on this figure is the calculated Pitot pressure distribution for



**Figure 6.13:** Experimental Pitot pressure (circles) and the calculated Pitot pressure with (solid line) and without (dashed line) a turbulent wall condition. The bars indicate one standard deviation of the experimental signal noise.

a nozzle simulation where the boundary layer is assumed to be completely laminar (the details of the laminar boundary layer simulation were the same as the turbulent boundary layer simulation, except for the exclusion of the turbulence model). The experimental Pitot pressure compares more favourably with the results of the turbulent flow simulation, and indicates that the assumption of turbulent boundary layer growth along the nozzle wall (made in Section 5.2.3) is valid.

The performance of the Mach 7 nozzle can be compared with a similar Mach 10 nozzle designed for the T4 free piston shock tube [114]. The Mach 10 nozzle was designed using the MOC/BL technique which, as discussed in Section 1.2, assumes that the boundary layer and core flow are uncoupled. A comparison of the experimental Pitot pressure profiles for the nozzles can be made by scaling a normalized Pitot pressure profile for the Mach 10 nozzle, to the mean normalized Pitot pressure level of the Mach 7 nozzle. The radii of the two nozzles can also be normalized by the respective nozzle exit radii,  $y_{max}$ . The comparison is shown in Fig. 6.14. The Pitot pressure profile for the Mach



**Figure 6.14:** Comparison of the Pitot pressure normalized by nozzle supply pressure for the optimized Mach 7 nozzle and the T4 Mach 10 nozzle.

10 nozzle was obtained from a high stagnation pressure shot (40 MPa) and it is, therefore, a representation of the highest quality test flow the nozzle can produce [114]. The Mach 7 Pitot pressure profile is significantly more uniform across the core flow region, which suggests that the optimization nozzle design technique is an improvement over the MOC/BL technique.

#### 6.5 Summary

The nozzle contour designed in Chapter 5 using the design tool presented in Chapters 2 & 3, was used to construct a nozzle for a small reflected shock tunnel at The University of Queensland. The test flow issuing from this nozzle was then assessed by performing Pitot pressure surveys to confirm the effectiveness of the design method. The Pitot

pressure survey across the exit plane of the nozzle showed that the standard deviation in Pitot pressure of the core flow was approximately 1.6%, which is significantly higher than estimated by the design calculations (0.05%), but still very good. It was suspected that the uniformity of the nozzle flow may be better than indicated by the experimental measurements because of the large amount of noise in the Pitot pressure signals. A possible source of the noise was suggested as being an acoustic oscillation within the Pitot probe cavity.

The maximum flow angularity of the exit core flow was estimated as being  $0.35^{\circ}$  using the results of a second Pitot pressure survey at an axial location 58.5 millimetres downstream of the nozzle exit plane. The downstream Pitot survey showed two distinct "humps" in the Pitot pressure profile at the edges of the core flow. A time accurate simulation of the unsteady nozzle starting process and the development of the test flow within the test section, showed that these humps were possibly due to unsteady test section wave interaction caused by the relatively high static pressure within the test section and dump tank prior to the shot.

# Design of a Shock Tunnel Nozzle with a Square Cross-Section

The use of square (or rectangular) cross-section nozzles to expand the test flow in wind tunnels is an attractive alternative to using axisymmetric nozzles because square cross-section nozzles do not have the same focusing characteristics that can magnify wall disturbances. Axisymmetric nozzles tend to focus any wall disturbance to the nozzle centre line. In contrast, square cross-section nozzles distribute wall disturbances laterally along lines parallel to the walls rather than being focused to a point (see Fig. 7.1). Subsequently,



Figure 7.1: Focusing of a wall disturbance in an (a) axisymmetric and (b) square cross-section nozzle.

square cross-section nozzles are often favoured for long nozzles that are built in sections (e.g. the 31 Inch Mach 10 wind tunnel at NASA Langley [150]). Core flow disturbances resulting from imprecise mating of sections, boundary layer transition, or other wall anomalies are not as pronounced at the exit plane of square cross-section nozzles compared to axisymmetric nozzles. Another benefit of square cross-section nozzles is the ease of inserting windows (into their flat walls) for optical diagnostics.

Despite these benefits, it is not common to see shock tunnel nozzles designed with square or rectangular cross-sections. One rectangular cross-section nozzle was designed and built for the T4 facility at The University of Queensland in 1989, however, the performance was poor. The nozzle was designed using the method of characteristics and a boundary layer correction, and included a boundary-layer bleed to control the mid-wall separation of the boundary layer.

In this chapter, a computational design study is carried out using the design tool discussed in Chapters 2 & 3, to ascertain (i) the feasibility of a Mach 7 square cross-section nozzle for the Small Shock Tunnel pulse facility (see Section 5.1 for a description of this facility), and (ii) the effectiveness of the computational design tool for designing square cross-section nozzles. The study consists of designing three square cross-section nozzles of varying length, and assessing the quality of the flow issuing from the exit planes. The design tool used for the design of the nozzles incorporated the three-dimensional implementation of sm3d, which is capable of modelling cross-flow separation and complex inviscid-viscous three-dimensional interactions. These effects are typically ignored in square cross-section nozzle design techniques based on the method of characteristics [62, 24, 78, 90, 221].

### 7.1 Review of Square Cross-Section Nozzle Design

In the past, square cross-section supersonic and hypersonic wind tunnel nozzles have been designed using an extension of the method of characteristics/boundary layer correction (MOC/BL) technique [62, 24, 78]. The method involved determining an inviscid nozzle wall surface and then correcting it for viscous effects with the addition of a local boundary layer displacement thickness. The inviscid wall contour is determined by first calculating an axisymmetric nozzle wall contour that produces uniform parallel test flow expanded to the desired Mach number using the method of characteristics. Streamlines that intersect the desired cross-sectional exit shape are then traced back upstream through the axisymmetric flow-field from the nozzle exit plane. The three-dimensional surface formed from these streamlines gives the desired inviscid nozzle shape, which is then corrected for boundary layer growth. The cross-sectional shape of the inviscid surface at all axial locations, except at the throat, deviates slightly from the prescribed shape at the exit plane of the nozzle. If the flow at the nozzle throat is uniform, then the cross-sectional shape at the throat is the same as the shape at the exit plane.

One of the earliest three-dimensional square cross-section nozzles designed using the method described above was the Mach 9.6 nozzle [24] for the 11 Inch Hypersonic Tunnel at NASA Langley. The surface of the nozzle was machined with the bowed cross-sections resulting from streamline tracing, and the inviscid contour was corrected for viscous effects by adding an average displacement thickness for a given cross-section. Surveys of the nozzle exit flow showed a uniform test core of 4 inches by 4 inches with a maximum variation in Mach number of 1.5% [2]. The manufacture of square cross-section nozzles was simplified in later applications of the design technique by making all the cross-sections square. This simplification was applied to the design of a Mach 10 nozzle for the 31 Inch wind tunnel at NASA Langley [90] and the Mach 4.7 and Mach 6 square
#### 7.1 Review of Square Cross-Section Nozzle Design

cross-section nozzles for the NASA Langley arc-heated scramjet test facility [221]. Flow surveys of these nozzles [151, 152, 221] have shown that the exit core flow is very uniform, where the variation in core flow Mach number for the Mach 4.7 and Mach 6 nozzles is approximately 2%, and for the Mach 10 nozzle less than 1%.

The flow surveys of the these square cross-section nozzles have also shown that there are large regions of separated boundary layer flow on the side walls of the nozzles. The 31 Inch Mach 10 nozzle and the Mach 6 nozzle for the scramjet test facility both produce very good test flows. However, the boundary layer developed along the side walls is separated at the exit plane and large pairs of counter-rotating vortices are present within the separated boundary layer, limiting the size of the test core. The vortices, with their cores aligned with the axial direction, are a result of three-dimensional cross-flow effects on the walls of the nozzle that are not modelled in the axisymmetric flow-field streamline tracing design method. Cross-flow occurs in square nozzles and on the flat side walls of two-dimensional nozzles (rectangular section), where a pressure gradient is established due to the uneven expansion between the corner and the centre-plane. In contoured square cross-section nozzles, where there is an initial convex expansion followed by a straightening concave expansion, there is an initial span-wise movement of the boundary layer flow towards the corners, then a reversal towards the mid-points of the wall as the corner static pressure increases after the wall contour inflection point. The span-wise movement of the boundary layer flow results in collisions of flow at the corners and at the wall midpoints. If the span-wise velocity is great enough, the colliding flow streams may cause the boundary layer to become separated, and pairs of counter-rotating vortices may form at the nozzle corners or wall mid-points [168].

Despite the presence of the large regions of separated boundary layers at the exit planes of the square cross-section nozzles discussed, the nozzles are recognised as being capable of producing test flow of high quality. This is a curious result given the highly three-dimensional nature of the exit flow and the simple axisymmetric flow-field streamline tracing method used to design the nozzles. A possible explanation for this result is that the effects of cross-stream separation on core flow quality are minimised by lengthening the nozzle. For a given exit flow Mach number, a longer nozzle will have a smaller wall-curvature. A smaller wall-curvature will then reduce the magnitude of the side wall pressure gradient that causes boundary layer separation. Also, the cross-stream pressure distribution at every axial location will become more uniform. The square cross-section nozzle flow static pressure distribution then becomes more like the axisymmetric nozzle flow. Hence, the axisymmetric design method becomes more accurate as the nozzle length is increased. This reasoning will be investigated in this chapter.

All of the square cross-section nozzles discussed above are in use (to the author's knowledge) on intermittent and continuous flow wind tunnels. Therefore, the nozzle

starting process is not a major concern, and the nozzle can be made long without significantly reducing the test time. However, the increased nozzle starting time associated with long nozzles becomes significant in pulse flow wind tunnels, where the test time is of the same order as the nozzle starting time [106]. Therefore, shorter nozzles are favoured with larger wall expansion angles [199, 115]. However, the discussion above suggests that the traditional methods used for designing square cross-section nozzles may not be suitable for short square cross-section nozzles because of the increased three-dimensional nature of the flow as the nozzle length is reduced. This chapter explores the feasibility of using a three-dimensional flow solver and an optimization algorithm to design square cross-section nozzles for pulse flow wind tunnels.

## 7.2 The Computational Configuration

Three square cross-section nozzles of varying length were designed for use in the Small Shock Tunnel facility (see Section 5.1). The shapes of the nozzle expansion contours were optimized for minimum core flow Mach number deviation from the design Mach number, and minimum core flow angularity at the nozzle exit planes. The design goals for the square cross-section nozzle core flows were (i) an exit Mach number of 7 with a variation of Mach number across the inviscid core at the exit plane of less than 0.01 (or 0.14 %), and (ii) a variation of flow angularity less than 0.016 degrees ( $\sim$  1 arc minute). These are the same goals used for the axisymmetric nozzle design in Section 5.2. Again, it should be emphasised that these design goals are "ideal" goals and are set high to improve the convergence of the optimization search algorithm; flow variations of this magnitude could not be measured in the facility.

Since the cross-section of square cross-section nozzles is bilaterally symmetric, only one quarter of each of the three nozzles was modelled. Each quarter section of the nozzles was defined as a continuous duct from the nozzle throat to the exit plane with four Bézier curves defining the edges of the nozzle box-section (see the grid bounding box in the middle of Fig. 2.14). One of the Bézier curve edges was defined as a straight line that was mapped to the *x*-axis. The other three Bézier curves defined the contoured walls of the nozzle, and the control points for these Bézier curves were used to define the optimization design variables.

The initial shapes for the three square cross-section nozzles were based on the optimized axisymmetric Mach 7 nozzle design discussed in Chapter 5. One of the initial square cross-section nozzle designs had the same length as the as the optimized axisymmetric nozzle (nominal length), and the other two nozzles had lengths that were half and double the length of the axisymmetric nozzle. The resulting lengths for the short, nominal and long nozzles were 185.5, 371 and 742 millimetres respectively. Each square cross-section nozzle shape was defined with Bézier curves consisting of 10 control points. The axial distribution of these control points for the nominal length nozzle is shown in Fig. 7.2. The axial coordinates correspond to the coordinates of the control points for



Figure 7.2: Definition of the wall contour for the nominal square cross-section nozzle .

the upstream and downstream Bézier curves defining the wall contour of the axisymmetric nozzle design (see sheet 4 and 6 of Appendix H). The initial y/z coordinates of the square cross-section Bézier control points were set to the radial coordinates used for the optimized axisymmetric nozzle.

The optimization problem was configured so that the position of the first three upstream Bézier points remained fixed and the radial position of the seven other Bézier control points were determined by the optimization algorithm. The coordinates of the control points were defined by the optimization design variables which were equal to the radial distance between consecutive Bézier control points as given by the following list:

$$dv[0] = Y_3 - 4.68$$
  

$$dv[1] = Y_4 - Y_3$$
  

$$dv[2] = Y_5 - Y_4$$
  

$$dv[3] = Y_6 - Y_5$$
  

$$dv[4] = Y_7 - Y_6$$
  

$$dv[5] = Y_8 - Y_7$$
  

$$dv[6] = Y_9 - Y_8$$
  
(7.1)

The objective function used for the square cross-section nozzle optimization, defined the variation of Mach number and flow angle along a line across the exit plane, parallel to the *z*-axis, extending from the centre of the nozzle to the edge of the core flow. The edge of the core flow was defined as the position along the sample line where the axial velocity component was equal to 99% of the centre line velocity (approximate edge of boundary layer). All of the computational cells along this line were used to evaluate the objective function which was defined as,

$$Obj(dv) = (f_{\theta} + f_M)^2 \quad . \tag{7.2}$$

The two functions defining the variation in flow angle,  $\theta$ , and the distribution in Mach number, were

$$f_{\theta} = \frac{\phi_{\theta}^2}{N} \sum_{j=1}^{N} (u_{z,j}/u_{x,j})^2$$

$$f_M = \frac{\phi_M^2}{N} \sum_{j=1}^{N} (M_{x,j} - M_{\text{design}})^2$$
(7.3)

where N denotes the number of cells coinciding with the sample line.

Two weighting parameters,  $\phi_{\theta}$  and  $\phi_M$ , were used to scale the functions  $f_{\theta}$  and  $f_M$  so that both functions evaluate to 1 or less if all of the cells within the core flow along the sample line satisfy the respective design goals. The weighting parameters are equal to the inverse of the design goals (or tolerances) such that,

$$\phi_{\theta} = \frac{1}{\tan(0.016)} = 3.58 \times 10^{3}$$

$$\phi_{M} = \frac{1}{0.01} = 10^{2}$$
(7.4)

Each of the three initial nozzle shapes were optimized using the Nelder-Mead simplex optimization algorithm [159] (see Chapter 3). The initial perturbations of the design variables that form the initial simplex at the start of the optimization algorithm were set to 1 millimetre for the first three design variables, and 2 millimetres for the remaining four design variables (see Eq. 7.1 for design variables). No constraints were placed on the design variables and no penalty functions were imposed on the objective function.

The flow data that was used to evaluate the objective function for a particular design was obtained from a flow solution calculated using the sm3d flow solver. A threedimensional adaptation of Baldwin & Lomax's turbulence model (see Section 2.9) was used to model the development of turbulent boundary layers along the nozzle walls from the nozzle throat. The inflow conditions at the nozzle throat were the same uniform inflow conditions used for the axisymmetric nozzle design calculations. These throat conditions were presented in Table 5.1.

The computational grids for each of the three square cross-section nozzles were composed of 20 cells in the y direction, 20 cells in the z direction and 1000 cells in the axial direction for the short and nominal nozzles (2000 cells for the long nozzle). The crossstream cells were equally clustered towards the nozzle walls and the symmetry planes using an exponential stretching function parameter of 1.05 (Eq. 2.105 was used for the clustering). Along the nozzle axis, cells were clustered towards the throat using an exponential stretching function parameter of 2.5 . It was recognised that a cross-stream discretization of 20 by 20 cells would result in a poor resolution of the boundary layer development, however, the computational time required to compute a flow solution for a higher grid resolution would have made the solution time for the optimization problem impractical. If a grid of  $80 \times 80 \times 4000$  was used to discretize the computational domain for the short nozzle, it was estimated that the optimization algorithm would take on the order of 140 days to converge to an optimal design solution using one processor of the SGI Origin (based on the results for the short square cross-section nozzle presented in the following section). This is not a practical design problem to solve using the current computational resources available at The University of Queensland.

The computational boundary conditions for the surfaces of the computational domain representing the nozzle wall were set to a no-slip isothermal condition at a temperature of 296 K. The remaining side surfaces were used as symmetry planes and the boundary conditions on these surfaces were set to reflective slip walls. A calorically perfect nitrogen model was used to model the thermodynamic behaviour of the test gas, and the flow was assumed to be chemically frozen. The numerical stability of the flow calculations was maintained with a CFL number of 0.3 and the computational convergence criteria for each marching slice was set as a maximum change in cell density of 0.01% between time steps.

#### 7.3 **Optimization Results**

The results of the three optimization problems are given in Table 7.1 where the CPU times are quoted for a single R10000 processor on a SGI Origin 2000 (see Appendix G). The optimization algorithm was terminated for each case when the variance of the

Nozzle Number of CPU time Objective

**Table 7.1:** Optimization results of the three square cross-section nozzle designs.

Nozzle	Number of	CPU time	Objective		
	iterations	hours	Initial	Optimized	
Short	189	54	$3.211 \times 10^{9}$	155331	
Nominal	190	72	$8.600 \times 10^6$	309	
Long	134	88	$1.385 \times 10^5$	1.2	

simplex objective function values fell below 0.1 (see Eq. 3.1). The optimization of the long, square cross-section nozzle was the only case where the objective function for the optimum nozzle shape evaluated to a value below 2, which indicated that some of the core flow cells had achieved the design goals. However, the maximum wall slope of the long nozzle was only  $5.7^{\circ}$ , compared to the maximum wall slopes of  $16.3^{\circ}$  for the short nozzle and  $10.9^{\circ}$  for the nominal length nozzle. The small wall angle of the long nozzle is not a favourable design quality for pulse facility nozzles because a nozzle with a small wall angle requires a longer time to establish a steady test flow, thus reducing the test time (see Section 5.1). A more desirable maximum wall expansion angle for pulse facility nozzles has been suggested as being within the range of 10 to 15 degrees [199, 241, 115, 125], which would put the optimum nozzle length somewhere between the lengths of the short and nominal nozzles.

The coordinates for the control points of the Bézier curves which define the edges of the initial and optimized square cross-section nozzle shapes are presented in Table 7.2. The corresponding axial coordinates of the control points for each of the three nozzles can

Control	Â	Initial $y/z$	Optimized $y/z$		
point			Short	Nominal	Long
p0	0.0000	3.50	3.50	3.50	3.50
p1	0.0135	3.50	3.50	3.50	3.50
p2	0.0270	4.48	4.68	4.68	4.68
p3	0.1105	12.00	9.91	9.42	10.70
p4	0.1644	16.72	11.22	14.73	15.39
p5	0.2722	25.92	18.57	23.79	23.65
рб	0.4340	33.75	23.35	30.62	33.37
p7	0.6092	37.29	27.35	34.59	39.72
p8	0.7978	41.01	28.89	39.51	40.08
p9	1.0000	41.80	33.39	42.54	45.16

**Table 7.2:** Coordinates of the control points defining the Bézier curves for the initial and optimized square cross-section nozzle shapes (coordinates in millimetres).

be determined from the parametric coordinate  $\hat{X}$ , where  $\hat{X} = x/L$  and L is the total length of each nozzle (see Section 7.2 for lengths). The control point coordinates can be used in the Bézier polynomial equation, Eq. 2.103, to determine the nozzle edge coordinates. Figure 7.3 shows the nozzle edge profiles for the initial and optimized nozzle designs. As would be expected, the side wall length at the exit plane of each nozzle increases with nozzle length to accommodate the growth of the boundary layer.

The profiles of the optimized nozzle designs are also shown in Fig. 7.4, where the axial and side wall lengths of all the designs have been normalized by the axial and max-



Figure 7.3: Wall profiles for the initial and optimized square cross-section nozzle shapes.

imum side wall length of the optimized short nozzle design. This figure shows that the normalized shapes of all the optimized nozzle designs are very similar, however, the optimized shape approaches the initial shape as the nozzle is lengthened. Since the initial



**Figure 7.4:** Wall profiles of the optimized square cross-section nozzle shapes normalized by the length and maximum radius of the optimized short nozzle design.

nozzle designs are based on an optimized axisymmetric nozzle design, this result suggests that the optimum square cross-section nozzle shape becomes less sensitive to the three-dimensional nature of the flow as the nozzle is lengthened.

An analysis of the flow generated by the optimized designs was undertaken by first performing a high resolution flow calculation for each of the optimized nozzle shapes. The high resolution computational domain for each of the square cross-section nozzles was discretized into  $80 \times 80$  cells in the cross-flow plane, and these cells were clustered equally to each wall and symmetry planes using a clustering parameter of 1.1. The domains for the short length nozzle and the nominal length nozzle were both discretized with 4000 cells axially, and the long nozzle was discretized with 8000 cells. A clustering parameter of 2.5 was also used to axially cluster the cells towards the nozzle throat. The other computational settings for the flow simulation were the same as those used in the flow solver for the low resolution optimization flow calculations. The high resolution flow solutions for the optimized short, nominal and long nozzle designs required 35.2, 37.3 and 77.3 CPU hours respectively to run to completion using one processor of the SGI Origin 2000.

The Mach contours of the flow solutions at the exit planes of the three optimized square cross-section nozzles are shown in Fig. 7.5. The distinguishing flow features in



**Figure 7.5:** Computed Mach contours at the exit plane of the optimized square cross-section nozzles. The flow solutions were calculated using high resolution grids. The Mach contours range from 0.15 to 7.30 in 0.15 steps.

common with all of the nozzle exit flows are the separated boundary layers at the midpoints of the nozzle walls. Separation at the mid-points of the walls in square cross-section nozzles has also been observed experimentally in the Mach 6 square cross-section nozzle for the NASA Langley arc-heated scramjet test facility [221], and in the Mach 10 nozzle for the 31 Inch wind tunnel at NASA Langley [151]. However, there is some evidence that suggests the tendency for boundary layer separation at the wall midline is reduced as the Mach number or expansion ratio of the nozzle is reduced. The flow-field survey of the Mach 4.7 square cross-section nozzle for the NASA Langley arc-heated scramjet test facility [221] only showed a slight thickening of the boundary layer around the mid-points of the walls at the exit plane. Also, a computational study of a Mach 2.4 slow-expansion square cross-section nozzle did not show any boundary layer separation at the wall mid-points [135].

Another feature shown in the Mach number contour plots, is boundary layer separation at the corners of the nominal length nozzle. As stated earlier, the separation at the corners of the nozzle is a result of the boundary layer separating in the early part of the expansion where the cross-stream flow direction of the boundary layer is towards the corners. This flow feature has also been observed in other computational studies of square cross-section nozzles [168, 135], particularly where the expansion rate in the early part of the nozzle is slow.

The reason why the nominal length nozzle exhibits boundary layer separation at the nozzle corners and the other designs do not, can be determined by examining the wall pressure gradients. Figure 7.6(a) shows how the cross-stream wall pressure gradient varies with length for all three nozzles. The pressure gradient was calculated by taking the ratio



**Figure 7.6:** (a) Average normalized wall pressure gradient across half the side walls of the optimized square cross-section nozzles and (b) optimized nozzles wall slope versus axial distance.

of the difference in static pressure at the nozzle corner and wall midline, and the crossstream distance from the corner to the wall midline. This ratio was then normalized by the average of the corner and midline static pressures. A positive pressure gradient indicates that the static pressure at the nozzle corner is greater than the static pressure at the wall mid-point. The negative pressure gradient that is responsible for the boundary layer separation at the corners of the nozzle, is seen to be higher over a larger axial distance for the nominal length nozzle compared to the other two nozzles. The tendency for the negative pressure gradient to cause boundary layer separation increases moving further downstream where the boundary layer has thickened, since there is a greater amount of low momentum fluid for the pressure gradient to act on. Therefore, the nominal length nozzle has a greater tendency to produce corner-separated flow.

Figure 7.6(b) shows the variation of wall slope as a function of axial distance for all three optimized nozzle shapes. An interesting feature of the optimized short nozzle is the flaring out of the last section of the nozzle. It is assumed that the optimizer has done this in an effort to minimise the pressure gradient across the walls at the exit plane and make the exit flow more uniform. The result of the flaring can be seen in the top part of Fig. 7.6 where there is a rapid drop in wall pressure gradient in the last 75 millimetres of the nozzle.

The magnitude of the wall pressure gradient, which is a function of wall slope or expansion rate, has a large effect on the magnitude of the vorticity associated with the exit flow boundary layers. A short, rapidly expanding nozzle develops a large pressure gradient on the nozzle walls which turns the flow more rapidly once it is entrained in the boundary layers. The effect of the wall pressure gradient can be seen in Fig. 7.7, which shows the cross-stream velocity vectors (i.e. only y and z velocity components) at the exit plane of each of the optimized nozzles. The short nozzle velocity vectors near the wall,



**Figure 7.7:** Cross-stream velocity vectors across the exit plane of the optimized square cross-section nozzles (every fourth vector is shown).

generally have a larger magnitude than the vectors for the other nozzles. They also appear to turn more rapidly either side of the wall mid-point in comparison to the velocity vectors associated with the longer nozzle shapes. To confirm this observation, the cross-stream vorticity of the flow across the nozzle exit planes was calculated, and the maximum axial vorticity levels were identified. The axial vorticity component,  $\omega_x$ , was calculated using,

$$\omega_x = \frac{\partial u_y}{\partial z} - \frac{\partial u_z}{\partial y} \quad . \tag{7.5}$$

For each of the nozzles, the locations of peak vorticity levels were very close to the nozzle walls either side of the wall mid-points. The peak vorticity values are shown in Table 7.3, along with the maximum nozzle expansion angles and the maximum transverse velocities at the nozzle exit planes. The short square cross-section nozzle clearly has a greater

 Table 7.3: The maximum computed axial vorticity at the exit planes of the optimized square cross-section nozzle designs.

Nozzle	Maximum	Maximum transverse $u$		Maximum
	wall angle	m/s	% of $u_{\text{axial max.}}$	vorticity, $s^{-1}$
Short	16.2°	263	12.9	$540 \times 10^{3}$
Nominal	10.8°	178	8.7	$296 \times 10^{3}$
Long	$5.7^{\circ}$	84	4.1	$67 \times 10^{3}$

maximum axial vorticity and maximum transverse velocity than the longer nozzles. This increase appears to be a result of the greater wall slope, which in turn increases the wall cross-stream pressure gradient as noted previously.

A square cross-section nozzle that develops a high level of known vorticity within the boundary layer and a uniform test core, may be beneficial for "direct connect" scramjet experiments where the nozzle exit flow is fed directly into the scramjet combustor. The ingestion of the non-uniform nozzle wall flow into a scramjet combustor, could simulate the ingestion of the non-uniform flow generated by the vehicle forebody which is an inherent part of the design. Testing could also be carried out by ingesting the more uniform flow in engine testing [221]. Therefore, there may be some benefit in having a short nozzle if the nozzle can be designed so that the exit flow is uniform to within acceptable limits.

The variation in computed Mach number and flow angle across a line from the centre of the nozzle to the mid-point of the wall at the exit plane for each of the optimized nozzle shapes is plotted in Fig. 7.8. The data shown in these plots are from the high resolution flow simulations of the optimized nozzle designs. Also shown on these plots are the design tolerances for Mach number and flow angularity. The sampled data line goes through the thickest part of the separated boundary layer, so it gives a good indication of the test core size for each of the nozzles. The test core for the short nozzle is substantially smaller than the other two nozzles primarily because the mean Mach number across the test core is less than the mean for the other two nozzles. A lower exit Mach number



**Figure 7.8:** Exit plane distribution of (a) Mach number and (b) flow angularity along a line from the centre of the flow to the wall centre.

corresponds to a smaller exit area. The size of the test cores for the two longer nozzles are very similar as is the mean Mach number across the test core. This result is consistent with isentropic expansion theory.

It is interesting to note that the separated boundary layer region is the greatest for the long nozzle rather than the short nozzle which exhibits a much higher degree of vorticity within the boundary layer. The thickening of the separated boundary layer regions seems to be a result of boundary layer growth and length over which the wall pressure gradient acts, rather than the magnitude of the wall pressure gradient. Figure 7.6 shows that the positive wall pressure gradient causing boundary layer flow reversal is clearly the smallest for the long nozzle. However, this gradient acts over a large distance compared to the other nozzles, and results in a thicker separated boundary layer.

The plots in Fig. 7.8 show that none of the nozzle shapes produce core flows with exit Mach number variation and flow angularity that are within the design tolerances. However, the magnitude of the variation tends to decrease with nozzle length. The high resolution simulation of the long optimized nozzle shape showed that the flow angularity of the core flow was very good, and the variation in Mach number from the mean core flow level was also very good. However, the mean core flow Mach number was substantially different to the design goal. This result is contrary to the value of the objective function for the optimized long nozzle shape, which indicates that at least a small proportion of the core flow should be at a Mach number of 7. This inconsistency was investigated by plotting the exit flow Mach number distribution for the low resolution simulation of the optimized long nozzle design, against the distribution calculated using two grids of a higher resolution. These plots are shown in Fig. 7.9. The large difference in the size of the core



**Figure 7.9:** Exit plane distribution of Mach number along a line from the centre of the nozzle to the wall midline for grids of increasing resolution (from high resolution simulation).

flow between the low resolution simulation and the higher resolution simulations, is due to the separated boundary layer region not being accurately resolved in the low resolution simulation and subsequently, the mean core flow Mach number being reduced. The plot shows that the Mach number distribution for the low resolution simulation does indeed have a mean level close to the design Mach number as indicated by the objective function. Therefore, the discrepancy is a result of the grid resolution. The mean level of the Mach number being different to the design Mach number is generally not a major concern for experimental purposes. A more important concern is the variation in flow quantities across the core flow. Figure 7.10 shows the variation in Mach number and flow angularity obtained from the high resolution flow solutions for the initial and optimized long nozzle designs. Clearly the flow angularity of the initial shape was improved substantially by optimization with a low resolution grid, and the low variation in Mach number for the initial shape was maintained through optimization. It is likely that performing the long nozzle optimization again with a high resolution grid (although impractical because of the computational requirements) would result in only an improvement in the mean value of the Mach number, since the optimized nozzle test core flow variation in Mach number and flow angularity is already small.



**Figure 7.10:** (a) Mach number, and (b) flow angularity profile at the long nozzle exit flow plane, along a line from the centre of the flow to the wall centre.

#### 7.4 Summary & Recommendations

Optimization of all the initial nozzle shapes was shown to decrease the Mach number variation and maximum flow angularity of the nozzle exit plane core flow. The computed exit plane core flow Mach number variation and maximum flow angularity for all of the optimized nozzle shapes is summarised in Table 7.4 (based on high resolution flow calculations). Also shown in this table are the maximum wall expansion angles. As indicated

**Table 7.4:** The core flow Mach number variation and maximum flow angularity for the optimized square cross-section nozzles.

Nozzle	Mach No. variation	Maximum	Maximum	
	(% of mean)	angularity	wall angle	
Short	7.03	1.21°	16.2°	
Nominal	0.96	0.23°	10.8°	
Long	0.48	0.11°	5.7°	

earlier (see Section 7.3), the maximum wall expansion angle is significant because it indicates how suitable the nozzle designs are for use as a shock tunnel nozzle. Shock tunnel nozzles are generally designed with maximum expansion angles ranging between  $10^{\circ}$  to  $15^{\circ}$  to ensure that the nozzle starting process is relatively fast [199, 115].

The optimized long nozzle shape has a maximum wall expansion angle that is considerably lower than that recommended for a shock tunnel nozzle and, even though the flow quality is similar to the exit flow quality of the optimized axisymmetric nozzle in Chapter 5, it is unlikely that the nozzle design would be suitable for a shock tunnel nozzle. The optimized nominal length nozzle is more suitable with a maximum wall expansion angle that is at the lower end of the suggested range. However, the exit flow variation for this nozzle is double the variation for the long nozzle and poorer than the optimized axisymmetric nozzle of Chapter 5. The flow variation appears to get rapidly worse as the length of the nozzle is reduced further as indicated by the results for the short nozzle. Therefore, it appears that a contoured square cross-section nozzle that produces high quality flow and is suitable for use in a shock tunnel, is not physically realisable for the flow condition studied here.

The main reason why it was not possible to reduce the exit plane flow variation to acceptable levels (i.e. as good as, or better than, that achieved for the axisymmetric nozzle in Chapter 5) for nozzles with high maximum expansion angles, was because the three-dimensional nature of the core flow increases as the wall expansion angle of the nozzle increases. Increasing the wall expansion angle increases cross-stream pressure gradients at the nozzle walls and results in an uneven expansion across the cross-stream plane.

The cross-stream pressure gradients for the long nozzle were significantly smaller than those for the shorter nozzles (see Fig. 7.6) and, as a result, the nozzle shape could be optimized to produce exit flows with a significantly lower flow variation. Also, since the cross-stream pressure gradients were low for the long nozzle, the initial shape derived from the optimized axisymmetric nozzle shape of Chapter 5 showed a low flow variation at the nozzle exit to begin with (see Fig. 7.10). This is the reason why the method used in the past to design long square cross-section nozzles for continuous and intermittent wind tunnels has been successful (see Section 7.1). However, the flow through any contoured square cross-section nozzle design design with a more uniform exit flow will result by using a design tool that can model these gradients, rather than using a classical method that is based on streamline tracing through an axisymmetric flow-field.

As indicated previously, it was not possible to optimize the short and nominal length square cross-section nozzle shapes to produce exit flow with a flow variation equal to, or better than, that produced by the axisymmetric design of Chapter 5. However, the designs may have been improved if the computational grid used to perform the computations for the optimization was of a higher resolution. A higher resolution grid would have allowed

the solver to resolve the cross-stream pressure gradients and fine detail of the flow more accurately. These effects become more influential on the core flow as the nozzle length is shortened. Currently, using a higher resolution grid in the design tool is not practical with the available computer processor technology but, in the future, it may be worthwhile investigating whether the nominal length nozzle design can be improved to an extent that it can be used for a shock tunnel nozzle.

Before concluding this chapter, two other important modelling issues are identified that may be relevant for future design work. Firstly, in the current study, the flow entering the nozzle through the nozzle contraction from the nozzle supply region was assumed to be inviscid such that no boundary layers formed on the nozzle contraction walls. For square cross-section contractions, this assumption can have a significant effect on the nozzle exit flow since large cross-stream pressure gradients are present in square cross-section contractions. These pressure gradients can create separated boundary layer regions and form vortices at the nozzle contraction corners, which then propagate downstream into the nozzle expansion [135]. Secondly, the boundary layer flow within the nozzles designed in the current study was assumed to be turbulent with no points of transition. If possible, boundary layer transition should be avoided on expanding nozzle surfaces because the transition can create unwanted disturbances in the test flow [3, 135]. It may be preferable to induce boundary layer transition prior to the flow entering the nozzle throat so that the entire expansion wall boundary layer is turbulent. Designing a nozzle wall to account for boundary layer transition may compound the disturbances created by transition if the estimation of a transition point is incorrect.

## Conclusions

This thesis was concerned with the development and application of a computational design tool consisting of a numerically efficient parabolized Navier-Stokes flow solver and a Nelder-Mead optimization algorithm. The design tool was used to design (1) a complete axisymmetric Mach 12 scramjet engine flow path, (2) an axisymmetric Mach 7 nozzle for a shock tunnel, and (3) a square cross-section Mach 7 nozzle for a shock tunnel. These three design studies demonstrated that the new design tool can be used to improve the shape of aerodynamic bodies that experience multidimensional, high temperature, inviscid/viscous flow interactions. The design of these bodies historically required gross simplifying assumptions, which may be relaxed to some extent when using the present design tool.

Through the application of the design tool to the aforementioned design cases, many insightful discoveries and recommendations were made, which have already been discussed at the end of the respective chapters. The final chapter of this thesis is concerned with the conclusions made in regard to the design tool itself. Firstly, the computational flow solver is discussed, followed by the optimization algorithm. Some recommendations for further research into extending the capabilities of the design tool are also presented.

#### 8.1 Parabolized Navier-Stokes Flow Solver

The purpose of the parabolized Navier-Stokes flow solver was to accurately and quickly calculate the flow-fields of a candidate design. Selected flow quantities from these flow-field solutions were then used by the optimization algorithm to determine an incremental shape improvement in the pursuit of generating a desired flow-field. The aerodynamic applications of the design tool in this thesis required the flow solver to calculate high temperature, viscous, supersonic flow-fields. To this end, a computationally efficient space-marching scheme for integrating the parabolized Navier-Stokes (PNS) equations was used as the basis of the flow solver. Through the development of the flow solver, an emphasis was placed on using CFD techniques that were not overly complicated.

Finite-volume discretization was used in the flow solver to solve the integral form of the three-dimensional and axisymmetric PNS equations. A finite-volume approach was taken because it is inherently conservative and well suited to flows with discontinuities such as shocks. A time-dependent form of the integral equations was also used to explicitly march the cross-flow slices of finite volume cells forward in time to a steady state, before marching in space to the next downstream slice. The explicit time integration technique used to march flow slices forward in time was shown to be robust enough for computing complex three-dimensional flows as well as chemically reacting flows, where the fluid and chemical time scales are very disparate.

The cross-stream inviscid fluxes were calculated using a numerically efficient, low dissipation, upwind approximate Riemann solver, and a spatially third-order accurate monotone upstream-centred scheme for conservation laws (MUSCL) extrapolation. A minimum-modulus limiter was also used to suppress numerical oscillations around discontinuities such as shocks. The numerical scheme was shown to capture shocks adequately without solution dependent coefficients, and accurately resolve boundary layers because of the flux solver's inherent low dissipation. The ability to resolve boundary layers accurately was an important trait of the numerical scheme for the design cases considered in this thesis.

In an attempt to model the high temperature flow effects present in scramjet engines and shock tunnel nozzles, a thermodynamic equilibrium model and an Arrhenius finiterate reaction model were implemented in the flow solver. The thermodynamic equilibrium model was used to solve the equation of state for cases where the vibrational energy modes of the gas became excited, and the reaction model was used to determine the source terms in the PNS equations for multi-species chemically reacting flows in non-equilibrium. An approximately-coupled integration technique was used to solve for the chemical production terms in the PNS equations, and a Roe averaged ratio of specific heats was used in the approximate Riemann solver invariants to stabilise the chemically reacting flow calculations with variable specific heats. This numerical scheme for modelling high temperature thermochemical effects was shown to be numerically efficient and accurate within the bounds of applicability.

The highly separated boundary layers in the flows of high Mach number square crosssection nozzles motivated the inclusion of a three-dimensional turbulence model in the flow solver. The Baldwin & Lomax algebraic, two layer, eddy-viscosity model was used in preference to other models because of its simplicity and ease of application to threedimensional, right angle corner flows. The model also uses a length scale based on vorticity to calculate the outer layer turbulent viscosity, which is more appropriate for separated flows. Compressibility effects were also modelled by using a compressible damping term. The extent of the modelling capabilities and accuracy of the flow solver were demonstrated through the simulation results obtained for eight test cases, which were presented in Appendix E. Accompanying experimental data and results from other validated flow solvers agreed favourably with all of the test cases, indicating that the phenomenological models used in the flow solver were sufficiently accurate and had been implemented correctly. Execution times for the flow solver were shown to be largely dependent on the models and equations used to solve a particular flow case. Overall, the flow solver was sufficiently fast and accurate that it could be used as part of the objective function evaluation within the optimization procedure. For a single optimization study, many flow solutions need to be generated and fine distinctions need to be made between similar solutions as an optimum solution is approached.

## 8.2 Optimization Algorithm

The identification of design improvements for scramjet flow-paths and high Mach number nozzles is not a trivial task because of the many interrelated flow characteristics. An increasingly popular way of automating such design problems is to use an optimization algorithm to interpret relationships between the flow-field data and the aerodynamic shape, and to make improvements accordingly. An advantage of this design optimization approach is the independence of the optimization algorithm and the flow solver, making it possible to couple almost any flow solver with any type of optimization algorithm. In this thesis, a gradient-search Nelder-Mead optimization algorithm was coupled to the developed flow solver to form the design tool used for the supersonic/hypersonic design problems presented.

The Nelder-Mead optimization algorithm is a gradient-search algorithm that does not require the inversion of a sensitivity matrix to find an appropriate search direction. The search direction is found by evaluating and comparing the objective function evaluations at vertices of a simplex. Therefore, the algorithm functions without the evaluation of sensitivity derivatives that require the objective function to be continuously differentiable. This feature of the optimization algorithm was deemed necessary for the scramjet design case since shocks were present in the flow that may have caused the objective function to become discontinuously differentiable. A slope-based optimization algorithm was selected over a stochastic genetic algorithm because it was believed that the computationally intensive global-search capabilities of stochastic algorithms, such as genetic algorithms, would not be required. This proved to be true, since judicious selections of the initial designs and parametric studies performed prior to optimization ensured that the initial designs were close to the optimal design.

The number of CFD flow solutions (or objective function calls) required by the optimization algorithm to converge to an optimum design solution for the design cases presented in this thesis, was found to be dependent on the number of design variables used, the complexity of the flow being modelled, and the convergence criteria used. A recent study used the design tool discussed in this thesis to optimize the thrust produced by a two-dimensional scramjet thrust surface with three design variables [111]. The flow was modelled using the Euler equations and heat was simply added to the flow though a source term. For this problem, the Nelder-Mead optimization algorithm required only 35-45 flow solutions to be calculated before an optimum design was found. Conversely, the optimization of the square cross-section nozzle expansion surface for uniform exit flow in the current study required 190 flow solutions to find the optimum design, using the same optimization algorithm. Seven design variables were used to define the expansion surface, and the flow solver modelled a highly three-dimensional viscous flow. The variability in the number of flow solutions required by the optimization algorithm to converge to an optimum design makes performance comparisons with other optimization algorithms published in the literature difficult.

Despite the variability in the number of flow solutions required for convergence in the current study, the range and magnitude is typical of other studies published using gradient-based optimization algorithms [138, 191, 120]. Some gradient-based optimization studies using sensitivity derivatives have utilized simplified analysis techniques to substantially reduce the number of complete flow solutions required, however, these methods have only been used for nonreacting inviscid flows [22, 148].

A limitation of the Nelder-Mead gradient-search algorithm was demonstrated in the chapter concerned with the design of an axisymmetric shock tunnel nozzle contour. The algorithm was shown to be susceptible to converging to a local minima rather than the global minimum (or true optimum design) for initial nozzle shapes that were not similar to the optimized nozzle shape. The tendency for the optimization algorithm to converge to the global minimum may have been made more likely by modifying the objective function to include a centre line Mach number distribution for example. However, the behaviour of the algorithm converging to a local minima is typical of most gradient-search algorithms. To have a reasonable assurance that a converged design obtained from a gradient-search algorithm is the true optimum design, it may be necessary to start the design from various initial points as was done in this study. The parametric study performed for finding the optimal combustor length for the scramjet was also a useful exercise for identifying the design space containing the optimum design.

## 8.3 **Recommendations**

The differences between the actual flow generated by an optimized aerodynamic shape and the qualities of the flow claimed by the objective function for the optimized shape, are largely a result of the flow solver modelling limitations. In the current study, the flow solver was developed to an extent where many of the high temperature viscous flow effects present in the flow-fields of the aerodynamic bodies studied could be accurately modelled. However, as indicated throughout the discussions of these design cases, there is scope to develop the flow solver further to increase its accuracy and fidelity. The two most important areas of development indicated were a molecular diffusion model and a multi-species thermodynamic non-equilibrium model.

Gradient-search optimization algorithms, like the one used in the design tool presented in this thesis, are susceptible to local minima convergence for initial designs that are not similar to the optimal design. Therefore, design tools using gradient-search algorithms are generally not very effective when applied to problems where a good initial design is not determinable. One idea for removing this limitation would be to replace the gradient-search optimization algorithm with a stochastic algorithm such as a genetic algorithm, which has the capability of global-search. However, the penalty for having a global-search capability is a substantial increase in the number of flow solutions required to obtain an optimized design, and a corresponding increase in computation time. An alternative to choosing one optimization algorithm over another may be to formulate a hybrid algorithm, where a genetic algorithm is coupled to a gradient-search algorithm. In this hybrid algorithm, a genetic algorithm could be used initially to search the entire design space for the global minimum region. Then, a gradient-search algorithm could be used to perform the final convergence to the global minimum since it will converge faster than the genetic algorithm. This approach would utilise the best qualities of both classes of optimization algorithm.

# Axisymmetric Parabolized Navier-Stokes Equations

This appendix presents the integral form of the axisymmetric parabolized Navier-Stokes (PNS) equations which can be used in the sm3d flow solver as an alternative to the threedimensional PNS equations presented in Section 2.4. A full treatment of deriving the axisymmetric Navier-Stokes equations from the three-dimensional equations is given in [105]. The governing equations for axisymmetric flow presented in this reference can be written with the PNS assumptions applied for a multi-species gas (see section 2.4) as

$$\frac{\partial}{\partial t} \int_{\Omega} \mathbf{U} \mathrm{d}\Omega' + \oint_{S} y(\mathbf{F}_{\mathbf{i}} - \mathbf{F}_{\mathbf{v}}) \cdot \hat{\mathbf{n}} dS = \int_{\Omega} \mathbf{Q} \mathrm{d}\Omega' \quad , \tag{A.1}$$

in the axisymmetric control volume  $\Omega$  bounded by the surface S. The algebraic vector of dependent flow variables is

$$\mathbf{U} = \begin{bmatrix} f_i \rho \\ \rho u_x \\ \rho u_y \\ \rho E \end{bmatrix} , \qquad (A.2)$$

the inviscid flux vector is

$$\mathbf{F}_{\mathbf{i}} = \begin{bmatrix} f_i \rho u_x \\ \rho u_x^2 + \epsilon p \\ \rho u_y u_x \\ \rho E u_x + p u_x \end{bmatrix} \hat{i} + \begin{bmatrix} f_i \rho u_y \\ \rho u_y^2 + p \\ \rho u_z u_y \\ \rho E u_y + p u_y \end{bmatrix} \hat{j} \quad , \tag{A.3}$$

and the viscous flux vector is

$$\mathbf{F}_{\mathbf{v}} = \begin{bmatrix} 0\\0\\0\\0 \end{bmatrix} \hat{i} + \begin{bmatrix} 0\\\tau_{xy}\\\tau_{yy}\\u_x\tau_{xy} + u_y\tau_{yy} - q_y \end{bmatrix} \hat{j} \quad , \tag{A.4}$$

where  $(i = 1, 2, ..., N_s)$ .

The viscous stresses are given by

$$\tau_{xx} = \lambda \left( \frac{\partial u_y}{\partial y} + \frac{u_y}{y} \right) ,$$
  

$$\tau_{yy} = 2 \mu \frac{\partial u_y}{\partial y} + \lambda \left( \frac{\partial u_y}{\partial y} + \frac{u_y}{y} \right) ,$$
  

$$\tau_{xy} = \mu \frac{\partial u_x}{\partial y} = \tau_{yx} ,$$
(A.5)

(A.6)

where  $\mu$  is the first coefficient of viscosity. As before, this formulation of viscous stresses assumes negligible bulk viscosity. Care must be taken when evaluating the viscous stresses on the axis where y = 0. On this axis, all fluxes evaluate to 0 because of the y multiplier in the integral equation (A.1). The viscous heat fluxes are

$$q_x = 0$$
 and  
 $q_y = k \frac{\partial T}{\partial y}$ . (A.7)

The effective source term (containing the front and back interface contributions) is

$$\mathbf{Q} = \begin{bmatrix} \dot{\omega_i} \\ 0 \\ (p - \tau_{\theta\theta})A \\ q \end{bmatrix}$$
(A.8)

where

$$\tau_{\theta\theta} = 2\,\mu \frac{u_y}{y} + \lambda \left(\frac{\partial u_y}{\partial y} + \frac{u_y}{y}\right) \tag{A.9}$$

The volume,  $\Omega$ , used in the above equations, is the axisymmetric cell volume per unit radian defined as

$$\Omega = \frac{A \cdot y_{\text{cell}}}{2\psi} \quad , \tag{A.10}$$

where A is the area of the cell which is equivalent to the ZFace area in the threedimensional formulation,  $y_{cell}$  is the distance from the cell centre to the axis, and  $2\psi$  is the circumferential extent of the axisymmetric cell in radians (see Figure A.1).



Figure A.1: Axisymmetric finite volume cell.

# **Thermodynamic Data Coefficients**

This appendix presents the coefficients for the polynomial expressions in temperature that can be used to calculate equilibrium thermodynamic quantities for the predominant species present in the combustion of hydrogen in air (see Section 2.6.2 for details of polynomials). The data is based on the data presented in the NASP Technical Memorandum 1107 [163] (except for the Argon polynomial coefficients which were derived from the JANAF thermodynamic tables [41]) and is valid over a range of temperatures from 200 K to 6000 K. The data listed below is in the following format:

- Line 1 : species name or formula, data source
- Line 2 : molecular weight (g/mol), heat of formation/R at 298 K (J/mol),  $H_{298}^{\circ} H_0^{\circ}$  (J/mol), heat of formation at 0 K (J/mol)
- Line 3 : temperature range for first polynomial, number of coefficients for  $C_p$ , T exponents in polynomial for  $C_p$
- Line 4 : first five coefficients
- Line 5 : last three coefficients for  $C_p$ , integration constant for  $H^{\circ}/RT$  and  $S^{\circ}/R$ Repeat of lines 3,4,5 for the second temperature interval

```
Н2
                       GLUSHKO ET. AL. TABLES VOL 1, PART 2,1978,pp 31,32.
 2.01588 0.0000000e+00 -8.467e+03 0.0
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 4.07827381e+04 -8.00908919e+02 8.21460291e+00 -1.26969910e-02 1.75358386e-05
 -1.20284571e-08 3.36805269e-12 0.0000000e+00 2.68245215e+03 -3.04375206e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 5.60805609e+05 -8.37139111e+02 2.97532730e+00 1.25223484e-03 -3.74067336e-07
 5.93655676e-11 -3.60695230e-15 0.0000000e+00 5.33975192e+03 -2.20273775e+00
                      GLUSHKO ET. AL., VOL 1, PT 2, p18, 1978.
02
 31.99880 0.0000000e+00 -8.683e+03 0.0
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
-3.40523954e+04 4.80666522e+02 1.14879791e+00 4.18908582e-03 -4.97972664e-07
 -2.18455977e-09 1.09324947e-12 0.0000000e+00 -3.37336164e+03 1.83386032e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -1.05642070e+06 2.41123849e+03 1.73474238e+00 1.31512292e-03 -2.29995151e-07
 2.13144378e-11 -7.87498771e-16 0.0000000e+00 -1.73025987e+04 1.79886219e+01
```

```
CODATA, 1989. Woolley, JRNBS VOL 92, 1987, p 35.
H20
18.0152 -2.90848168e+04 -9.904e+03 -238.921e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -3.94795976e+04 5.75572946e+02 9.31783525e-01 7.22271043e-03 -7.34255377e-06
 4.95504081e-09 -1.33693246e-12 0.0000000e+00 -3.30397423e+04 1.72420529e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 1.03497195e+06 -2.41269814e+03 4.64611030e+00 2.29199858e-03 -6.83683125e-07
 9.42647001e-11 -4.82238112e-15 0.0000000e+00 -1.38428678e+04 -7.97814507e+00
Н
                       CP/R=2.5. D0(H2)=36118.3 INVCM FROM HERZBERG.
 1.00794 2.62191552e+04 -6.197e+03 216.035e+03
    200.000 \ 1000.000 \ 1 \ 0.0 \ 0.0 \ 0.0 \ 0.0 \ 0.0 \ 0.0 \ 0.0 \ 0.0
 2.50000000e+00 0.0000000e+00 0.0000000e+00 0.0000000e+00 0.0000000e+00
 0.0000000e+00 0.0000000e+00 0.0000000e+00 2.54737802e+04 -4.46682853e-01
  1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 5.83910541e+01 -1.75634127e-01 2.50020546e+00 -1.19464572e-07 3.64899146e-11
-5.57727760e-15 3.35299119e-19 0.0000000e+00 2.54748952e+04 -4.48145562e-01
                       NSRDS-NB3 3, 1975. TEMPERATURE CUT-OFF & FILL.
15.99940 2.99680919e+04 -6.725e+03 246.79e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -8.66965739e+03 1.70920430e+02 1.90998257e+00 1.16784527e-03 -1.33343162e-06
 8.14268965e-10 -2.05401114e-13 0.0000000e+00 2.83540783e+04 8.71749100e+00
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 2.56765883e+05 -7.16872793e+02 3.30458292e+00 -4.22037538e-04 1.02051997e-07
-9.23795699e-12 2.62330613e-16 0.0000000e+00 3.38387627e+04 -5.75914912e-01
OН
                       GLUSHKO ET. AL. TABLES VOL 1, PART 2,1978, pp 37,38.
17.00734 4.73184830e+03 -9.172e+03 38.390e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -1.99883669e+03 9.30002687e+01 3.05081739e+00 1.52951129e-03 -3.15785360e-06
 3.31540674e-09 -1.13874911e-12 0.00000000e+00 3.23956828e+03 4.67405553e+00
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 1.01738037e+06 -2.50992485e+03 5.11648390e+00 1.30529703e-04 -8.28425761e-08
 2.00645654e-11 -1.55697743e-15 0.00000000e+00 2.04445349e+04 -1.10126733e+01
                       Hills, JCP v81,1984,p4458, Jacox, JPCRD, v17,1988,p303.
HO2
 33.00674 1.50965000e+03 -10.003e+03 5.01e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -7.59820983e+04 1.32927014e+03 -4.67665097e+00 2.50807553e-02 -3.00617570e-05
 1.89530203e-08 -4.82765013e-12 0.00000000e+00 -5.80883977e+03 5.19320281e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
-1.81124399e+06 4.96477618e+03 -1.04118720e+00 4.56103964e-03 -1.06210433e-06
 1.14489981e-10 -4.76481209e-15 0.0000000e+00 -3.19543890e+04 4.06806872e+01
H2O2
                       GLUSHKO, V 1, PT 1, pp 121-123, 1978.
34.01468 -1.63425145e+04 -10.853e+03 -129.808e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
-9.27586636e+04 1.56425231e+03 -5.97386681e+00 3.27006364e-02 -3.93124226e-05
 2.50858212e-08 -6.46315831e-12 0.0000000e+00 -2.49376400e+04 5.87571627e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 1.48904547e+06 -5.16993250e+03 1.12812684e+01 -8.00903641e-05 -1.82603198e-08
 6.95596790e-12 -4.83164774e-16 0.0000000e+00 1.41766201e+04 -4.65027729e+01
                      GLUSHKO ET. AL. TABLES VOL 2, PART 2, 1979, P 29.
CO
 28.01040 -1.32936276e+04 -8.671e+03 -113.81e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 1.48902869e+04 -2.92225259e+02 5.72445933e+00 -8.17613952e-03 1.45688636e-05
 -1.08773353e-08 3.02790632e-12 0.00000000e+00 -1.30306962e+04 -7.85915227e+00
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 4.61913914e+05 -1.94468052e+03 5.91664175e+00 -5.66420706e-04 1.39879544e-07
-1.78765558e-11 9.62080176e-16 0.0000000e+00 -2.46577231e+03 -1.38739551e+01
```

```
CO2
                       GLUSHKO ET. AL. CONSTANTS VOL 2, PART 1,1979, P 31-33.
 44.00980 -4.73281047e+04 -9.364e+03 -393.151e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 4.57405495e+04 -5.73011080e+02 5.00228634e+00 3.34006355e-03 -1.44460953e-06
 1.43751814e-10 1.75471937e-14 0.0000000e+00 -4.55373204e+04 -5.38599026e+00
  1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 1.15460081e+05 -1.78337370e+03 8.28644239e+00 -8.98356945e-05 4.26107946e-09
-1.81443266e-12 6.29130739e-16 0.0000000e+00 -3.91191002e+04 -2.64894238e+01
HNO
                       GLUSHKO ET. AL. VOL 1, PT 1,1978,p307. Jacox, 1988,p301.
 31.01408 1.22716582e+04 -9.988e+03 102.501e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
-6.85805047e+04 9.55633317e+02 -6.02692635e-01 8.00240256e-03 -6.65096915e-07
 -3.66313541e-09 1.78137330e-12 0.0000000e+00 6.43311018e+03 3.04962314e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -5.79796556e+06 1.94638589e+04 -2.15393271e+01 1.79834139e-02 -4.97880662e-06
 6.40176414e-10 -3.14462271e-14 0.0000000e+00 -1.10475800e+05 1.81959523e+02
                      GLUSHKO ET. AL. CONSTANTS VOL 1, PART 1,1978,p 292.
NO2
 46.00554 4.11247012e+03 -10.186e+03 35.93e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -5.64446389e+04 9.63636013e+02 -2.43620842e+00 1.92819349e-02 -1.87513061e-05
 9.14921401e-09 -1.77857778e-12 0.00000000e+00 -1.54949598e+03 4.06880767e+01
   1000.000 \quad 6000.000 \quad 7 \quad -2.0 \quad -1.0 \quad 0.0 \quad 1.0 \quad 2.0 \quad 3.0 \quad 4.0 \quad 0.0
 7.21538492e+05 -3.83321546e+03 1.11402049e+01 -2.23832673e-03 6.54839992e-07
-7.61220796e-11 3.32880923e-15 0.0000000e+00 2.50289180e+04 -4.30554999e+01
NO
                      GLUSHKO ET.AL. VOL 1, PT 2, p212, 1978
 30.00614 1.09765939e+04 -9.192e+03 89.775e+03
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 -1.13950869e+04 1.52905406e+02 3.43619274e+00 -2.68337801e-03 8.50453157e-06
 -7.70266072e-09 2.39192360e-12 0.0000000e+00 9.10090386e+03 6.70279386e+00
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 2.22923252e+05 -1.28721634e+03 5.43159665e+00 -3.64540455e-04 9.85484169e-08
 -1.41284573e-11 9.36437114e-16 0.0000000e+00 1.74864669e+04 -8.48487386e+00
                      NSRDS-NBS 3, 1975. TEMPERATURE CUT-OFF.
N
 14.00674 5.68500128e+04 -6.197e+03 470.82e+03
    2.50000000e+00 0.0000000e+00 0.0000000e+00 0.0000000e+00 0.0000000e+00
 0.0000000e+00 0.0000000e+00 0.0000000e+00 5.61046378e+04 4.19390885e+00
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 7.98383717e+04 -8.41344705e+01 2.33948210e+00 3.02865813e-04 -1.75861226e-07
 4.05061583e-11 -2.69675007e-15 0.00000000e+00 5.68237747e+04 5.03074884e+00
N2
                      GLUSHKO ET. AL. TABLES VOL 1, PT 2, p 207, 1978.
 28.01348 0.0000000e+00 -8.670e+03 0.0
    200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 2.21034481e+04 -3.81841578e+02 6.08266513e+00 -8.53081161e-03 1.38462951e-05
 -9.62567763e-09 2.51967544e-12 0.0000000e+00 7.10837479e+02 -1.07599032e+01
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 5.87702841e+05 -2.23921563e+03 6.06686971e+00 -6.13957913e-04 1.49178026e-07
-1.92307120e-11 1.06193594e-15 0.0000000e+00 1.28319075e+04 -1.58661574e+01
                      JANAF Tables
AR
 39.948 0.0000000e+00 -6.197e+03 0.0
    100.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 0.0000000e+00 0.0000000e+00 2.50003007e+00 0.0000000e+00 0.0000000e+00
 0.0000000e+00 0.0000000e+00 0.0000000e+00 -7.45342362e+02 4.37973116e+00
   1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0
 0.0000000e+00 0.0000000e+00 2.50003007e+00 0.0000000e+00 0.0000000e+00
 0.0000000e+00 0.0000000e+00 0.0000000e+00 -7.45342362e+02 4.37973116e+00
```

## **Finite-Rate Chemistry Models**

In order to simulate the hydrogen/air combustion process within a scramjet engine, a finite-rate reaction model needs to be implemented as part of the computational solver. Many models have been proposed for the hydrogen/air reaction mechanism over the last 30 years. These range in complexity from simple two reaction global models [183], to comprehensive reaction models such as the model presented by Oldenborg *et al.* [163] which consists of 31 reactions and 15 species. Generally, the accuracy of the more complex reaction models is superior to the simpler models, however, the more complex reaction models for hydrogen combustion in air are reviewed and assessed by analysing the results of a simple one-dimensional combustion flow calculation. An efficient reaction model is then selected for use in the optimization flow calculations presented in Chapter 4 and is further modified to improve its predictive performance. A listing of all reaction models assessed is given at the back of this appendix.

#### C.1 Finite-Rate Model for Scramjet Combustion

Reaction models for hydrogen and air can be broadly classed into two groups; (i) models involving reactions of hydrogen and oxygen only, and (ii) models including reactions of nitrogen and other trace elements present in air.

Reaction models that include nitrogen are important for accurately simulating the ignition delay time in high temperature flows (combustor flows at flight Mach numbers > 12) where nitrogen starts to dissociate and combine with atomic oxygen to form nitric oxide and nitrogen dioxide [102, 198]. Nitrogen reaction models become even more important at higher temperatures where large concentrations of nitrous radicals and molecules such as N, NO, and HNO form. The formation of these species can have a major influence on the heat release of the combustion reaction. In the scramjet design study of Chapter 4, the temperature of the pre-combustion flow was thought to be high enough to form small amounts of nitric oxide and nitrogen dioxide of high enough concentrations to effect the ignition delay. However, the maximum combustor temperature ( $\approx 3500$  K) was thought not to be high enough to produce large amounts of N, NO and HNO since nitrogen starts to dissociate appreciably at approximately 4000 K. Therefore, since the accurate calculation of ignition delay times was not a major concern with the current study, the investigation of combustion models was limited to those involving only hydrogen and oxygen.

Four hydrogen/oxygen reaction models were considered for implementation into the flow solver to be used for optimization:

- Rogers & Chinitz's 9-species, 23-reaction model [183] (excluding ozone reactions)
- Drummond's 9-species, 18-reaction model [55]
- Bittker & Scullin's 9-species, 15-reaction model [29]
- Evans & Schexnayder's 7-species, 8-reaction model [61]

The reaction paths and reaction rate data associated with each model are presented at the end of this appendix. All the reaction models include the same 9 species  $H_2$ ,  $O_2$ ,  $H_2O$ , OH, H, O,  $HO_2$ ,  $H_2O_2$ , and  $N_2$  (nitrogen only acts as a third body and does not dissociate) except for the model of Evans & Schexnayder which excludes  $HO_2$  and  $H_2O_2$ . In addition to these four models, Rogers & Chinitz's very efficient two-step global model describing the combustion of hydrogen in air [183] was also considered. However, the range of applicability of this model is limited and it produces extremely large disparity in the time scales of numerical problems. Since the flow solver that was used in this study employs explicit time marching that could not efficiently cope with such a large disparity, the model was discarded.

Each of the four reaction models were assessed by analysing the results of a onedimensional combustion flow calculation through a one metre long duct. The inflow conditions for the duct simulations were approximately the same as the core flow conditions at the exit plane of the optimized inlet discussed in Section 4.3.2 and are presented below:

$$\rho = 0.2704 \text{ kg/m}^3 \quad u = 3302 \text{ m/s} \quad e = 1.0315 \times 10^6 \text{ J/kg}$$
  
 $p = 101.3 \text{ kPa} \quad T = 1300 \text{ K} \quad M = 4.7$ 

The composition of the air used for the one-dimensional simulations differed slightly from the composition used for the inlet simulations. Argon was omitted from the composition leaving only nitrogen and oxygen with mass fractions of 0.7686 and 0.2314 respectively, where the mass of the argon was made up with extra nitrogen. A stoichiometric amount of hydrogen was uniformly added at a cross-stream flow plane 1 millimetre downstream of the inflow plane. The hydrogen was added to the flow through the source terms of the Euler equations which were used to model the flow (PNS equations without viscous terms). The hydrogen was added to the flow with an injection velocity of 3302 m/s and at a temperature of 800 K.

A set of four flow calculations were performed using each reaction model in turn. The computational domain for the flow calculations was discretized into 10000 cells, uniformly distributed along the 1 metre reaction length. Each of the four flow calculations used a CFL number of 0.4 to maintain numerical stability, except for the calculation using the Drummond reaction model. This reaction model was numerically stiffer than the others and required the CFL number to be set to 0.2 to maintain stability. The time-integration convergence criteria for all of the flow calculations was set to a total mass residual of 0.01%. The run times for each flow calculation using one processor or the Origin 2000 computer are presented in Table C.1, and selected distributions of computed flow data are shown in Fig. C.1. All of the reaction models produced similar results except for the model by Evans & Schexnayder which over-estimated the ignition delay

 Table C.1: Computation times for the one-dimensional combustion simulations using various combustion models.

Mechanism	No. of	No. of	CFL	CPU Time
	reactions	species		(sec)
Rogers & Chinitz, 1983 [183]	23	9	0.4	226.0
Drummond, 1988 [55]	18	9	0.2	411.3
Bittker & Scullin, 1972 [29]	15	9	0.4	214.3
Evans & Schexnayder, 1980 [61]	8	7	0.4	160.4



Figure C.1: Results from one-dimensional combustion simulation.

time and had a slower rate of heat release. However, the flow simulation using the smaller reaction model of Evans & Schexnayder was considerably faster than the next fastest simulation.

Also shown on the temperature distribution plot is the estimated ignition delay length using the empirical relation of Huber *et al.* [96] which was shown earlier in Eq. 4.3. This relation has been shown to give good approximations of ignition delay times that are computed using complex reaction models that incorporate nitrogen dissociation [56]. The computed ignition delay length is almost identical to the ignition delay length estimated using the Rogers & Chinitz model (which does not include nitrogen dissociation). Therefore, it can be argued that reactions involving nitrogen and nitrogen radicals do not have a strong influence on the ignition delay at this condition. Studies performed by others using similar conditions also support this conclusion [198, 102].

On the basis of computational efficiency, the reaction model by Evans & Schexnayder appeared to be the most appealing model to use in the optimization study for the scramjet combustor/thrust surface design. However, the distribution of heat release following ignition using this reaction model is significantly different to the other models examined. In the other three models, the heat release distribution is very similar. Under-estimating the rate of heat release may result in an under-estimation of the propulsive efficiency of the scramjet combustor/thrust surface. It was thought that, if the model by Evans & Schexnayder could be modified to give a similar heat distribution to the other models without an appreciable increase in the computational time required for a flow solution, the model would have sufficient accuracy and efficiency to be used in the optimization study.

The poor modelling of heat distribution with the reaction model of Evans & Schexnayder is primarily due to the absence of the reactions involving the radical hydroperoxyl (HO<sub>2</sub>). Fast three body recombination reactions involving HO<sub>2</sub> have been identified as contributors to the heat release process in hydrogen combustion in air [83]. Therefore, the HO<sub>2</sub> radical was added to the reaction model of Evans & Schexnayder to improve the heat release modelling capabilities. Two of the most important reactions involving HO<sub>2</sub> that provide a reaction path for the release of heat [102] were also added to the reaction model. The reactions used were 4 and 14 from the Rogers & Chinitz reaction model which are shown below:

$$H + O_2 + M \iff HO_2 + M$$
 (C.1)

$$H + HO_2 \iff 2OH$$
 (C.2)

The first reaction is a very fast third body reaction that produces  $HO_2$  from molecular oxygen and atomic hydrogen. The  $HO_2$  is then converted to hydroxyl by the second reaction. The hydroxyl radicals then react with the molecular hydrogen to form water,

#### C.1 Finite-Rate Model for Scramjet Combustion

thereby releasing heat into the flow. The addition of these reactions corrects the heat release distribution modelling deficiencies of the Evans & Schexnayder reaction model, however, it does not affect the ignition delay. Although a very accurate estimation of the ignition delay length was not a major concern of this study, the original Evans & Schexnayder reaction model estimates an ignition delay length that is nearly twice as long as the Rogers & Chinitz model.

The reason for the poor prediction of ignition delay when using the Evans & Schexnayder reaction model, is the absence of hydrogen peroxide  $(H_2O_2)$  from the reaction model. The hydrogen peroxide radical is only important for ignition and does not contribute significantly to the heat release process [163]. Adding sufficient reactions involving  $H_2O_2$  to the Evans & Schexnayder reaction model in order to correct the ignition delay time was not pursued. Making this addition would have increased the complexity of the reaction model to the size of the Bittker & Scullin model and the computational efficiency of the model would have been lost.

Apart from the hydrogen peroxide reactions, another reaction that has also been identified as important for low temperature ignition [102] which is included in the Evans & Schexnayder reaction model is the reaction

$$O_2 + H \longleftrightarrow OH + O$$
 . (C.3)

By changing the rate coefficients of this reaction, the Evans & Schexnayder model can be easily modified to correct the ignition delay time for the design condition without any loss in computational efficiency. The original forward rate equation for this reaction was determined by Baulch *et al.* [21] as  $k_f = 2.2 \times 10^{14} \exp(-8455/T)$  with an uncertainty of  $\pm 50\%$  for the temperature range 300 to 2000 K. By trebling the coefficient A to  $6.6 \times 10^{14}$ , the rate of hydroperoxyl radical production can be increased and hence the ignition delay time reduced. The original rate coefficient for this reaction in the Evans & Schexnayder model was replaced with the modified coefficient and the analysis problem was re-run using the modified reaction model.

The results of the simulation using the modified reaction model are shown in Fig. C.2. The modified Evans & Schexnayder reaction model shows a significant improvement in the heat release distribution and ignition delay time. The flow simulation time for the modified model was 186.4 seconds which is only a 16 % increase in computational time compared to the original model and is still significantly less than the simulation time of the other reaction models. The modified Evans & Schexnayder reaction model was selected as the reaction model to be used in the scramjet combustor/thrust surface design optimization because of its computational efficiency and enhanced accuracy.



**Figure C.2:** Results of a one-dimensional combustion tube simulation where the Evans & Schexnayder reaction model has been modified.
# C.2 Model Listings

Reaction		Reaction	Reaction rate variables		
number			$A_j$	$N_j$	$\theta$ , K
1	$H_2 + M$	$\longleftrightarrow H + H + M$	$5.5 \times 10^{18}$	-1.0	51987
2	$O_2 + M$	$\longleftrightarrow O + O + M$	$7.2 \times 10^{18}$	-1.0	59340
3	$H_2O + M$	$\longleftrightarrow \mathrm{OH} + \mathrm{H} + \mathrm{M}$	$5.2 \times 10^{21}$	-1.5	59386
4	OH + M	$\longleftrightarrow O + H + M$	$8.5 \times 10^{18}$	-1.0	50830
5	$H_2O + O$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$5.8 \times 10^{13}$	0.0	9059
6	$H_2O + H$	$\longleftrightarrow OH + H_2$	$8.4 \times 10^{13}$	0.0	10116
7	$O_2 + H$	$\longleftrightarrow \mathrm{OH} + \mathrm{O}$	$2.2 \times 10^{14}$	0.0	8455
8	$H_2 + O$	$\longleftrightarrow OH + H$	$7.5 \times 10^{13}$	0.0	5586
Third body efficiencies for all the termolecular reactions are 1.0					

Table C.2: Hydrogen and oxygen reaction model from Evans & Schexnayder [61].

 Table C.3: Hydrogen and oxygen reaction model from Bittker & Scullin [29].

Reaction	Re	action	Reaction rate variables		
number			$A_j$	$N_{j}$	$\theta$ , K
1	$H_2 + O_2$	$\longleftrightarrow OH + OH$	$1.00 \times 10^{13}$	0.0	21653
2	$\mathrm{H} + \mathrm{O}_2$	$\longleftrightarrow OH + O$	$1.25 \times 10^{14}$	0.0	8208
3	$H_2 + OH$	$\longleftrightarrow H_2O + H$	$2.19 \times 10^{13}$	0.0	2593
4	$\mathrm{O}+\mathrm{H}_2$	$\longleftrightarrow \mathrm{OH} + \mathrm{H}$	$1.74 \times 10^{13}$	0.0	4759
5	$\mathrm{O} + \mathrm{H}_2\mathrm{O}$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$5.75 \times 10^{13}$	0.0	9064
6	H + OH + M	$\longleftrightarrow H_2O + M$	$7.50 \times 10^{23}$	-2.6	0
7	2H + M	$\longleftrightarrow H_2 + M$	$1.00 \times 10^{18}$	-1.0	0
8	$\mathrm{H} + \mathrm{O}_2 + \mathrm{M}$	$\longleftrightarrow HO_2 + M$	$1.59 \times 10^{15}$	0.0	-504
9	$\mathrm{OH} + \mathrm{HO}_2$	$\longleftrightarrow H_2O + O_2$	$6.00 \times 10^{12}$	0.0	0
10	2O + M	$\longleftrightarrow O_2 + M$	$1.38 \times 10^{18}$	-1.0	171
11	$\mathrm{H} + \mathrm{HO}_2$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$7.00 \times 10^{13}$	0.0	0
12	$\mathrm{O} + \mathrm{HO}_2$	$\longleftrightarrow OH + O_2$	$6.00 \times 10^{12}$	0.0	0
13	$2HO_2$	$\longleftrightarrow H_2O_2 + O_2$	$1.80 \times 10^{12}$	0.0	0
14	$H_2 + HO_2$	$\longleftrightarrow H_2O_2 + H$	$9.60 \times 10^{12}$	0.0	12086
15	$\mathrm{H}_{2}\mathrm{O}_{2} + \mathrm{M}$	$\longleftrightarrow 2OH + M$	$1.17 \times 10^{17}$	0.0	22912
Т	he third-body ef	ficiencies are all 1.0	except for re	actions	
(6) 4.0 for $M = H_2$ , 1.6 for $M = O_2$ , 20.0 for $M = H_2O$ , 1.6 for $M = N_2$ ,					
(7) 5.0 for $M = H_2$ , 2.0 for $M = O_2$ , 15.0 for $M = H_2O$ , 2.0 for $M = N_2$ ,					
(8) 5.0 for $M = H_2$ , 2.0 for $M = O_2$ , 32.5 for $M = H_2O$ , 2.0 for $M = N_2$ ,					
(15) 2.3 fc	or $M = H_2, 0.78$ t	for $M = O_2$ , 6.0 for	$\mathbf{M}=\mathbf{H}_{2}\mathbf{O},6.6$	5 for M	$= H_2O_2,$

Reaction	ŀ	Reaction	Reaction ra	ate var	iables	
number			$A_j$	$N_j$	$\theta$ , K	
1	$H_2 + O_2$	$\longleftrightarrow OH + OH$	$0.170 \times 10^{14}$	0.0	24219	
2	$\mathrm{H} + \mathrm{O}_2$	$\longleftrightarrow OH + O$	$0.142 \times 10^{15}$	0.0	8249	
3	$\mathrm{OH} + \mathrm{H}_2$	$\longleftrightarrow H_2O + H$	$0.316 \times 10^{8}$	1.8	1524	
4	$\mathrm{O}+\mathrm{H}_2$	$\longleftrightarrow \mathrm{OH} + \mathrm{H}$	$0.207 \times 10^{15}$	0.0	6916	
5	OH + OH	$\longleftrightarrow H_2O + O$	$0.550 \times 10^{14}$	0.0	3521	
6	$\mathrm{H} + \mathrm{OH} + \mathrm{M}$	$\longleftrightarrow H_2O + M$	$0.221 \times 10^{23}$	-2.0	0	
7	H + H + M	$\longleftrightarrow H_2 + M$	$0.653 \times 10^{18}$	-1.0	0	
8	$\mathrm{H} + \mathrm{O}_2 + \mathrm{M}$	$\longleftrightarrow HO_2 + M$	$0.320 \times 10^{19}$	-1.0	0	
9	$\mathrm{HO}_2 + \mathrm{OH}$	$\longleftrightarrow H_2O + O_2$	$0.500 \times 10^{14}$	0.0	503	
10	$\mathrm{HO}_2 + \mathrm{H}$	$\longleftrightarrow H_2 + O_2$	$0.500 \times 10^{14}$	0.0	352	
11	$\mathrm{HO}_2 + \mathrm{H}$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$0.199 \times 10^{15}$	0.0	905	
12	$HO_2 + O$	$\longleftrightarrow OH + O_2$	$0.500 \times 10^{14}$	0.0	503	
13	$\mathrm{HO}_2 + \mathrm{HO}_2$	$\longleftrightarrow H_2O_2 + O_2$	$0.199 \times 10^{13}$	0.0	0	
14	$\mathrm{HO}_2 + \mathrm{H}_2$	$\longleftrightarrow H_2O_2 + H$	$0.301 \times 10^{12}$	0.0	9406	
15	$H_2O_2 + OH$	$\longleftrightarrow HO_2 + H_2O$	$0.102 \times 10^{14}$	0.0	956	
16	$\mathrm{H}_{2}\mathrm{O}_{2}+\mathrm{H}$	$\longleftrightarrow OH + H_2O$	$0.500 \times 10^{15}$	0.0	5030	
17	$H_2O_2 + O$	$\longleftrightarrow OH + HO_2$	$0.199 \times 10^{14}$	0.0	2968	
18	$\mathrm{H}_{2}\mathrm{O}_{2} + \mathrm{M}$	$\longleftrightarrow OH + OH + M$	$0.121 \times 10^{18}$	0.0	22886	
Th	Third body efficiencies for all the termolecular reactions are 1.0					

 Table C.4: Hydrogen and oxygen combustion reaction model by Drummond [55].

Reaction	]	Reaction	Reaction ra	ate var	iables
number			$A_j$	$N_{j}$	$\theta$ , K
1	$O_2 + M$	$\longleftrightarrow O + O + M$	$0.720 \times 10^{19}$	-1.0	59340
2	$H_2 + M$	$\longleftrightarrow H + H + M$	$0.550 \times 10^{19}$	-1.0	51987
3	$H_2O + M$	$\longleftrightarrow H + OH + M$	$0.520 \times 10^{22}$	-1.5	59386
4	$\mathrm{H} + \mathrm{O}_2 + \mathrm{M}$	$\longleftrightarrow HO_2 + M$	$0.230 \times 10^{16}$	0.0	-403
5	$H_2O_2 + M$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH} + \mathrm{M}$	$0.120 \times 10^{18}$	0.0	22900
6	O + H + M	$\longleftrightarrow \mathrm{OH} + \mathrm{M}$	$0.710 \times 10^{19}$	-1.0	0
7	$H_2O + O$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$0.580 \times 10^{14}$	0.0	9059
8	$H_2 + OH$	$\longleftrightarrow H_2O + H$	$0.200 \times 10^{14}$	0.0	2600
9	$O_2 + H$	$\longleftrightarrow OH + O$	$0.220 \times 10^{15}$	0.0	8455
10	$H_2 + O$	$\longleftrightarrow \mathrm{OH} + \mathrm{H}$	$0.750 \times 10^{14}$	0.0	5586
11	$H_2 + O_2$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$0.100 \times 10^{14}$	0.0	21641
12	$\mathrm{H} + \mathrm{HO}_2$	$\longleftrightarrow H_2 + O_2$	$0.240 \times 10^{14}$	0.0	350
13	$H_2 + O_2$	$\longleftrightarrow H_2O + O$	$0.410 \times 10^{14}$	0.0	25400
14	$\mathrm{H} + \mathrm{HO}_2$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$0.240 \times 10^{15}$	0.0	950
15	$H_2O + O$	$\longleftrightarrow H + HO_2$	$0.580 \times 10^{12}$	0.5	28687
16	$\mathrm{O} + \mathrm{HO}_2$	$\longleftrightarrow OH + O_2$	$0.500 \times 10^{14}$	0.0	504
17	$\mathrm{OH} + \mathrm{HO}_2$	$\longleftrightarrow O_2 + H_2O$	$0.300 \times 10^{14}$	0.0	0
18	$\mathrm{H}_2 + \mathrm{HO}_2$	$\longleftrightarrow H_2O + OH$	$0.200 \times 10^{14}$	0.0	12582
19	$\mathrm{HO}_2 + \mathrm{H}_2$	$\longleftrightarrow H + H_2O_2$	$0.730 \times 10^{12}$	0.0	9400
20	$H_2O_2 + H$	$\longleftrightarrow OH + H_2O$	$0.320 \times 10^{15}$	0.0	4504
21	$\mathrm{HO}_2 + \mathrm{OH}$	$\longleftrightarrow O + H_2O_2$	$0.520 \times 10^{11}$	0.5	10600
22	$\mathrm{HO}_2 + \mathrm{H}_2\mathrm{O}$	$\longleftrightarrow OH + H_2O_2$	$0.280 \times 10^{14}$	0.0	16500
23	$\mathrm{HO}_2 + \mathrm{HO}_2$	$\longleftrightarrow H_2O_2 + O_2$	$0.200 \times 10^{13}$	0.0	0
Th	ird body efficier	ncies for all the termoled	cular reactions	are 1.0	)

 Table C.5: Hydrogen and oxygen combustion reaction model by Rogers & Chintz [183].

Reaction	Reaction		Reaction r	ate var	iables	
number			$A_i$	$N_i$	$\theta, K$	
1	$OH + H_2$	$\longleftrightarrow H + H_2O$	$2.16 \times 10^8$	1.51	1726	
2	$H + O_2$	$\longleftrightarrow O + OH$	$1.91 \times 10^{14}$	0.0	8273	
3	$O + H_2$	$\longleftrightarrow H + OH$	$5.06 \times 10^{4}$	2.67	3166	
4	$\mathrm{H} + \mathrm{HO}_2$	$\longleftrightarrow H_2 + O_2$	$2.5 \times 10^{13}$	0.0	349	
5	$\mathrm{H} + \mathrm{HO}_2$	$\longleftrightarrow \mathrm{OH} + \mathrm{OH}$	$1.5 \times 10^{14}$	0.0	505	
6	$\mathrm{O} + \mathrm{HO}_2$	$\longleftrightarrow OH + O_2$	$2.0 \times 10^{13}$	0.0	0	
7	$\mathrm{OH} + \mathrm{HO}_2$	$\longleftrightarrow H_2O + O_2$	$2.0 \times 10^{13}$	0.0	0	
8	$\mathrm{H} + \mathrm{O}_2 + \mathrm{M}$	$\longleftrightarrow HO_2 + M$	$8.0 \times 10^{17}$	-0.8	0	
9	$\mathrm{H} + \mathrm{OH} + \mathrm{M}$	$\longleftrightarrow H_2O + M$	$8.62 \times 10^{21}$	-2.0	0	
10	H + H + M	$\longleftrightarrow H_2 + M$	$7.3 \times 10^{17}$	-1.0	0	
11	$\mathrm{H} + \mathrm{O} + \mathrm{M}$	$\longleftrightarrow \mathrm{OH} + \mathrm{M}$	$2.6 \times 10^{16}$	-0.6	0	
12	O + O + M	$\longleftrightarrow O_2 + M$	$1.14 \times 10^{17}$	-1.0	0	
13	OH + OH	$\longleftrightarrow O + H_2O$	$1.5 \times 10^{9}$	1.14	0	
14	OH + OH + M	$\longleftrightarrow H_2O_2 + M$	$4.73 \times 10^{11}$	1.0	-3206	
15	$OH + H_2O_2$	$\longleftrightarrow H_2O + HO_2$	$7.0 \times 10^{12}$	0.0	722	
16	$O + H_2O_2$	$\longleftrightarrow OH + HO_2$	$2.8 \times 10^{13}$	0.0	3220	
17	$\mathrm{H} + \mathrm{H}_2\mathrm{O}_2$	$\longleftrightarrow H_2 + HO_2$	$1.7 \times 10^{12}$	0.0	1900	
18	$\mathrm{H} + \mathrm{H}_2\mathrm{O}_2$	$\longleftrightarrow H_2O + OH$	$1.0 \times 10^{13}$	0.0	1800	
19	$HO_2 + HO_2$	$\longleftrightarrow H_2O_2 + O_2$	$2.0 \times 10^{12}$	0.0	0	
20	$\rm CO + OH$	$\longleftrightarrow CO_2 + H$	$4.4 \times 10^{6}$	1.5	-373	
21	O + NO	$\longleftrightarrow N + O_2$	$3.80 \times 10^{9}$	1.0	20820	
22	$O + N_2$	$\longleftrightarrow$ N + NO	$1.82 \times 10^{14}$	0.0	38370	
23	H + NO	$\longleftrightarrow \mathrm{N} + \mathrm{OH}$	$1.70 \times 10^{14}$	0.0	24560	
24	H + NO + M	$\longleftrightarrow HNO + M$	$2.17 \times 10^{15}$	0.0	-300	
25	O + NO + M	$\longleftrightarrow NO_2 + M$	$3.31 \times 10^{10}$	1.0	-4522	
26	H + HNO	$\longleftrightarrow$ H <sub>2</sub> + NO	$1.26 \times 10^{13}$	0.0	2000	
27	O + HNO	$\longleftrightarrow OH + NO$	$5.0 \times 10^{11}$	0.5	1000	
28	OH + HNO	$\longleftrightarrow$ H <sub>2</sub> O + NO	$1.26 \times 10^{12}$	0.5	1000	
29	$H + NO_2$	$\longleftrightarrow OH + NO$	$3.5 \times 10^{14}$	0.0	740	
30	$O + NO_2$	$\longleftrightarrow O_2 + NO$	$1.0 \times 10^{13}$	0.0	300	
31	$HO_2 + NO$	$\longleftrightarrow OH + NO_2$	$2.09 \times 10^{12}$	0.0	-240	
Third body efficiencies for all the termolecular reactions are						
	2.5 for $M = H_2$ , 1	6.25 for $M = H_2O$ , 3	$3.8 \text{ for } \mathbf{M} = \mathbf{C}$	$O_2$ ,		
	ar	nd 1.0 for all other M	1.			

Table C.6: NASP chemistry model for hydrogen combustion in air [163].

# **Lennard-Jones Potentials**

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	Substance	$\sigma, \check{\mathrm{A}}$	$\epsilon/k_B$
Air	Air	3.711	78.6
CO	Carbon monoxide	3.690	91.7
$\mathrm{CO}_2$	Carbon dioxide	3.941	195.2
Η	Hydrogen	2.070	37.0
$H_2$	Hydrogen	2.827	59.7
OH	Hydroxide	3.147	79.8
$H_2O$	Water (gas)	2.800	260.0
$H_2O_2$	Hydrogen peroxide	4.196	289.3
$HO_2$	Hydroperoxo	3.068	168.0
NO	Nitric oxide	3.470	119.0
Ν	Nitrogen	3.798	71.4
$N_2$	Nitrogen	3.798	71.4
$NO_2$	Nitrogen oxide	3.798	71.4
HNO	Nitrosyl hydride	3.798	71.4
$N_2O$	Nitrous oxide	3.828	232.4
0	Oxygen	3.050	106.7
$O_2$	Oxygen	3.467	106.7
Ar	Argon	3.42	124.0

Table D.1: Lennard-Jones 12-6 Potentials for various gases [174, 40].

# APPENDIX **E**

# **Test Cases**

The parabolized Navier-Stokes solver, *sm3d*, described in Chapter 2 was used to solve a set of eight test case flow problems, which are presented in this Appendix. The computational results for these test cases are compared with experimental and computational results from the published literature and show that the phenomenological models that were implemented into the solver were done so correctly. The variety of the test cases demonstrates that the solver is a robust, versatile and efficient flow solver for a variety of supersonic and hypersonic flows in all dimensions of space. Computation execution times are shown for each test case at the end of the Appendix, where the times are quoted for running the problems on a single processor of a Silicon Graphics Origin 2000 Rack (see Appendix G). This computer is currently the primary super-computer at The University of Queensland. These timing results show that the discretization and integration techniques used, were adequate for computing complex flows in a reasonable amount of time, thus making the solver practical for implementation in a design optimization algorithm.

Each test case is presented with a brief description of the problem, a listing of the computational setup used for the problem, and a discussion of the computational results. In order to make the description of the computational setup as succinct as possible, a listing of the parameter file and computation macros is presented, which were used by the flow solver at run time to configure the problem. The parameter file contains integration information, grid size and geometry, and the free-stream inflow condition. A line by line description of each entry in the parameter file is given in Appendix F. The computation macros define the type of simulation to be performed and the clustering of the computational grid.

A brief synopsis of the test cases presented in this Appendix is given below before discussing the details and results of each case:

E.1 The first test case was a flat plate boundary layer. This is a simple case that demonstrates the solver's ability to correctly resolve laminar boundary layers despite the Mach number being less than 1 for a significant part of the boundary layer. The

pressure splitting of Vigneron *et al.* [228] was also shown to be correctly applied and does not compromise the accuracy of the solution.

- **E.2** The second test cases consisted of modelling boundary layer/shock interactions for hypersonic flow past a compression corner. This case demonstrates the solver's ability to accurately resolve viscous boundary layers, and shows that it is capable of adequately capturing shocks without any user tuning.
- **E.3** Cross-flow separation of a boundary layer on the leeward side of a cone at an angle of attack was simulated in the third case. The cone flow is highly three-dimensional and exhibits a high degree of inviscid and viscous interaction. The successful flow calculation demonstrates the robustness of the solver.
- **E.4** The accuracy of the solver for estimating cross-flow separation was further tested in the fourth test case, where supersonic flow over two intersecting compression wedges was simulated. The wedges generate embedded shocks that interact with the boundary layers forming on the surfaces of the wedges and cause downstream separation.
- **E.5** The versatility of the B-Spline surfaces was demonstrated in the fifth test case by simulating the flow through a complex three-dimensional scramjet design. Combustion was simulated in the scramjet by adding heat through an energy source term in the governing equations.
- **E.6** Combustion was then accurately modelled in the sixth case by employing the solver's algorithms for modelling finite-rate chemical reactions and thermodynamic equilibrium. The finite-rate kinetics of hydrogen burning in air was simulated in the supersonic flow of a constant area duct. Explicit time stepping based on a finite-rate reaction time scale was shown to be stable and practical.
- E.7 The solver's algebraic turbulence model of Baldwin & Lomax [20] was exercised in the seventh test case by simulating the turbulent flow over a two-dimensional flap. The test case shows that the simple algebraic turbulence model of Baldwin & Lomax can produce reasonable approximations of viscous fluxes within turbulent boundary layers in the presence of a high degree of inviscid and viscous flow interaction.
- E.8 The final test case tests the solver's axisymmetric implementation of the parabolized Navier-Stokes equations by simulating the supersonic viscous flow over a cylinder. The good comparison of the simulation results with the results of a spectral collocation boundary layer algorithm verifies that the parabolized Navier-Stokes equations were implemented correctly.

### E.1 Flat Plate Boundary Layer

A simple case to test the implementation of the PNS equation set for modelling viscous flow, is a two-dimensional flat plate laminar boundary layer as shown in Fig. E.1. The case chosen consists of a 1.0 m flat plate aligned with a uniform Mach 2 flow. The gas was considered calorically perfect with  $\gamma = 1.4$ , R = 287 J/kg/K and a constant Prandtl number of 0.72. The computational domain, as shown in Fig. E.2, was shaped to include the leading-edge interaction shock (LEIS). The domain was divided into  $1000 \times 100$  cells



Figure E.1: Boundary layer along a flat plate with M = 2.0 and  $Re_L = 1.65 \times 10^5$ 



Figure E.2:  $1000 \times 100$  grid joining the cell centres (every 5th cell in the x-direction shown).

and the dimension calculation macro switch was set to two-dimensions (DIMENSION 2). The cells were clustered towards the plate surface with a clustering value of 1.01 and also towards the inlet plane with a clustering value of 1.1 (see Section 2.14).

The supersonic free-stream conditions of

$$\begin{split} \rho &= 0.0404 \text{ kg/m}^3, \quad u_x = 597.3 \text{ m/s}, \quad u_y = u_z = 0.0 \text{ m/s}, \\ p_\infty &= 2574 \text{ Pa}, \quad T_\infty = 222 \text{ K}, \quad T_{\text{wall}} = 222 \text{ K}, \\ M &= 2, \quad Re_L = 1.65 \times 10^5 \end{split}$$

were applied at the inlet plane. The South boundary condition, or plate surface, was set to be a no-slip wall with a constant temperature of 222 K. The East and West boundaries were set to solid walls with inviscid (slip) tangency conditions. The correct setting of the East & West boundaries is not essential when the two-dimensional macro is set since they are automatically set regardless of the user settings. The North boundary was set to a supersonic inflow condition.

All of this flow data and integration data is shown in the parameter file as:

```
VISCOUS Flat Plate Boundary Layer Flow
1001
                             case_id
0.25
       350 0.0001
                             CFL, max_t_steps, tolerance
2 7 0.8
                             Xorder, i_supress, p_safety
0.0 0.001 1.0 1000
                             Xi_0, dXi, X_max, max_x_steps
0.005
                             dXi_plot
1
                             slice_ident
100 2
                             nny, nnz
0 10
                             smooth_grid, smooth_iter
1 3 5 3
                             bc_N, E, S, W
222.0 222.0 222.0 222.0
                             Twall_N, E, S, W
0.0404 597.3 0.0 0.0 1.59285e5 free-stream rho, ux, uy, uz, e
0 0 1
                             use_B_spline, Bezier_box, 2d format
2
                             np
0.0 0.0
                             0 A
0.0 0.06
                               В
1.0 0.0
                             1 A
1.0 0.7
                               В
```

The macros of the header file are:

#define	DIMENSION	2
#define	VISC	1
#define	TURB	0
#define	CHEM	0
#define	FROZEN	0
#define	ADD_HEAT	0
#define	N_SP	1
#define	N_RE	1
#define	BETA_X_START	1.1
#define	BETA_X_END	0.0
#define	BETA_Y_TOP	0.0
#define	BETA_Y_BOTTOM	1.01
#define	BETA_Z_LEFT	0.0
#define	BETA_Z_RIGHT	0.0
#define	TYPE_of_GAS	PERF_AIR_14



Figure E.3: Pressure contours for the flat plate.

A pressure contour plot of the solution produced by the solver is shown in Fig. E.3. The only apparent feature is the weak shock propagating into the flow from the leading edge of the plate. However, a boundary layer develops along the plate and attains a total thickness of approximately 5 mm by the end of the plate. Figure E.4 compares the x-velocity and temperature profiles at x = 0.9415 m with profiles computed by a highly accurate boundary layer algorithm which is based on a spectral collocation method [172]. There is agreement to within 1.4% for velocity between the two solutions which, together with the LEIS resolution, verifies that the numerical scheme correctly captures the weak shock and resolves the viscous and heat fluxes.



**Figure E.4:** Comparison of the *sm\_3d* solution (circles) with a spectral solution (solid line). (a) x-velocity profile at x = 0.9415 m; (b) temperature profile at the same location.

# E.2 Hypersonic Flow Past a Compression Corner

The second test case consisted of simulating two-dimensional hypersonic flow past a compression corner which exhibits shock and boundary layer interaction. The problem consists of a flat plate connected to a  $15^{\circ}$  ramp in Mach 15 free-stream flow as shown in Fig. E.5.



Figure E.5: flow-field and grid for a hypersonic compression corner.

The inflow conditions are,

$$\begin{split} \rho_\infty &= 4.832 \times 10^{-4} \, \mathrm{kg/m^3}, \ u_x = 2401.56 \, \mathrm{m/s}, \ u_y = u_z = 0.0 \, \mathrm{m/s}, \\ p_\infty &= 10 \, \mathrm{Pa}, \quad T_\infty = 72.2 \, \mathrm{K}, \quad T_{\mathrm{wall}} = 297 \, \mathrm{K}, \\ M &= 14.1 \;, \ Re_L = 1.04 \times 10^5, \end{split}$$

and the horizontal plate length, L, is 0.439m. This flow-field was studied experimentally by Holden & Moselle in 1969 [91]. They made measurements of static pressure, heat transfer, and skin friction at various points along the flat plate and ramp. The predominant feature of the flow is the interaction of the leading edge incident shock forming off the start of the flat plate, and the shock induced by the 15° incline. These two shocks combine to form a single shock, a contact surface, and an expansion fan as shown in Fig. E.5.

The computational domain was discretized with  $2000 \times 90$  cells that were clustered towards the wall. The parameter file and calculation macros are as follows:

```
VISCOUS 2D Hypersonic laminar flow over a 15deg compression ramp
1002
                                 case_id
0.45 600 0.0001
                                 CFL, max_t_steps, tolerance
2 10 0.75
                                 Xorder, i_supress, p_safety
0.0 0.0005 1.0 2000
                                 Xi O, dXi, X max, max x steps
0.005
                                 dXi plot
1
                                 slice_ident
90
    2
                                 nny, nnz
0 0
                                 smooth_grid, smooth_iter
1
  3
      5
         3
                                 bc N, E, S, W
297.0 297.0 297.0 297.0
                                 Twall_N, E, S, W
4.832e-4 2401.56 0.0 0.0 51803.5 free-stream rho, ux, uy, uz, e
0 0 1
                                 B_spline, Bezier_box, 2d format
```

```
4
                                 np
0.000 0.0
                                  0 A
0.000 0.075
                                    В
0.439 0.0
                                  1 A
0.439 0.11495
                                    В
0.730 0.077973
                                  2 A
0.730 0.179
                                   В
0.900 0.1235
                                  2 A
0.900 0.203310
                                    В
#define DIMENSION
                       2
#define VISC
                       1
#define TURB
                       0
#define CHEM
                       0
                       0
#define FROZEN
#define ADD_HEAT
                       0
#define N_SP
                       1
#define N_RE
                       1
#define BETA_X_START
                       0.0
#define BETA_X_END
                       0.0
#define BETA_Y_TOP
                       0.0
#define BETA_Y_BOTTOM 1.04
#define BETA_Z_LEFT
                       0.0
#define BETA_Z_RIGHT
                       0.0
#define TYPE_of_GAS
                       PERF_AIR_14
```

Contour plots of Mach number and pressure for the flow solution over the compression ramp are shown in Fig. E.6. All of the flow features observed in the experiments by Holden & Moselle in 1969 [91] are well resolved in the computational solution. However, the computed shock formed by the compression corner shows a failing in the approximate Riemann solver used to calculate the inviscid fluxes (see Section 2.11.4). A small amount of non-physical oscillation can be seen propagating downstream of the shock in Fig. E.6(b), indicating that the Osher type approximate Riemann solver [107] is not very dissipative. A more dissipative flux solver could have been used to reduce this oscillation, however, the extra dissipation would cause inaccuracies within the boundary layer regions which is an important concern for this thesis.

The computational surface pressure,  $C_p$ , and heat transfer,  $C_h$ , coefficients were calculated along the wall for comparison with experimental data, where the coefficients are defined by the relations,

$$C_p = \frac{p}{\frac{1}{2}\rho_{\infty}u_{\infty}^2}, \quad \text{and} \quad C_h = \frac{k\frac{\partial T}{\partial y}\sec\theta}{\rho_{\infty}u_{\infty}[(e+\frac{p}{\rho}+\frac{u^2}{2})_{\infty}-(e+\frac{p}{\rho})_{\text{wall}}]}.$$
 (E.1)

The slope of the wall where each coefficient is evaluated is equal to the angle  $\theta$ . The calculated coefficients are compared with the experimental data of Holden and Moselle [91] in Fig. E.7.

A slight over-estimation relative to the experimental data is observed, however, this is consistent with other numerical simulations of the same problem [99, 126, 132, 202]. This difference has been attributed to incorrect free-stream data that was originally used by Holden & Moselle to compute the experimental coefficients [189]. Comparisons have been made using revised experimental data, where the free-stream conditions were recomputed using tunnel calibration data rather than using Pitot-tube measurements [190]. These comparisons show a substantial improvement in the agreement between the computed flow solution and experimental results.

The inability of the PNS equations to account for the upstream propagation of information in subsonic flow is demonstrated by the computed surface pressure coefficient at the corner of the ramp. The experimental coefficients show an increase in pressure before the ramp (x/L < 1.0) whereas the computational results do not show any increase until the ramp. The reason for the early increase in the experimental results is an upstream in-



**Figure E.6:** Contours of (a) Mach number and (b) static pressure for the 15° hypersonic compression ramp showing all the flow features described in Fig. E.5.



**Figure E.7:** Comparison of (a) computed pressure coefficients and (b) heat transfer coefficients (solid line) with Holden and Moselle's data [91](circles).

fluence of the ramp through the boundary layer, which is not physically realisable when using the PNS equations. Despite this inadequacy, the PNS solver produced reasonable results before and after the corner. Better agreement has been obtained for this test case in the corner region using a flow solver based on the full Navier-Stokes equations [190, 99].

# E.3 Viscous Hypersonic Flow Over a Cone at an Angle of Attack

The experiment performed by Tracy [225] was used as the third test case and involves viscous hypersonic flow over a cone at an angle of attack. The cone has a  $10^{\circ}$  half angle cone with an axial length of 0.3048 m and is positioned at a  $24^{\circ}$  angle of attack in Mach 7.95 flow (Fig. E.8).



Figure E.8: Cone at an angle of attack in a hypersonic flow.

The free-stream conditions are,

$$\begin{split} \rho_{\infty} &= 0.01254 \text{ kg/m}^3, \ u_x = 1083.57 \text{ m/s}, \ u_y = 482.44 \text{ m/s}, \ u_z = 0.0 \text{ m/s}, \\ p_{\infty} &= 199.4 \text{ Pa}, \quad T_{\infty} = 55.4 \text{ K}, \quad T_{\text{wall}} = 309.8 \text{ K}, \\ M &= 7.95, \ Re_L = 1.25 \times 10^6, \end{split}$$

and the wall temperature of the cone was fixed as 309.8 K. The cone axis is aligned with the x axis in computational space and the flow is angled at  $24^{\circ}$  to the cone axis in an upward direction (moving in a positive direction along the y-axis). The bottom half of the cone is the windward side and the top half the leeward side.

The high angle of attack results in a complex flow pattern forming around the cone making it a challenging problem for the solver. A conical shock forms around the body of the cone and weakens as the flow moves around to the leeward side. On the surface of the cone, a laminar boundary layer forms from the stagnated conditions on the windward side. As the boundary layer develops around the circumference of the cone, it thickens due to the expanding external flow that is accelerating to supersonic speeds. The two boundary layers meet at the top of the leeward side where they eventually separate as the flow moves down the length of the cone. The displacement thickness of the separation region grows in size and in doing so moves the leeward side of the conical shock further away from the surface. A secondary shock also forms around the separation region to provide the transition to subsonic speeds.

The computational grid used for this test case consisted of 50 cells normal to the surface and 56 cells around half of the circumference (from windward symmetry plane to leeward symmetry plane). Twenty thousand axial slices were used to discretize the computational domain axially, and these slices were clustered towards the nose. The cells were also clustered towards the surface. The grid was "wrapped" around half of the surface of the cone such that the outer windward corner of the grid was bounded by a 13° ray from the nose, and the leeward corner was bounded by a 35° ray. To avoid the grid discontinuity at the nose of the cone, the simulation was started at an axial position of x = 0.015 m. A yz cross-flow plane of the grid is shown in Fig. E.9.



Figure E.9: Cone computational grid for cross-flow plane (grid formed from cell centres).

Conical coordinates are used to display the profile of the grid where,

$$\theta_{y,z} = \frac{y,z}{R} \arctan \frac{R}{x}$$
 and  $R = \sqrt{y^2 + z^2}$ 

The parameter file and calculation macros for the cone problem are as follows:

```
Viscous 10 degree cone from Tracy 1963
1003
                                   case_id
0.25
       300 0.0001
                                   CFL, max_t_steps, tolerance
2 10 0.75
                                  Xorder, i_supress, p_safety
0.0 0.00005 1.0 20000
                                   Xi_0, dXi, X_max, max_x_steps
0.005
                                   dXi_plot
                                   slice_ident
1
50 56
                                   nny, nnz
0 10
                                   smooth_grid, smooth_iter
5 3 1 3
                                   bc_N, E, S, W
309.8 309.8 309.8 309.8
                                   Twall_N, E, S, W
0.01254 1083.57 482.44 0.0 39749.5 free-stream rho, ux, uy, uz, e
0 0 0
                                   B_spline, Bezier_box, 2d format
#define DIMENSION
                       3
#define VISC
                       1
#define TURB
                       0
#define CHEM
                       0
#define FROZEN
                       0
#define ADD_HEAT
                       0
#define N_SP
                       1
#define N_RE
                       1
#define BETA_X_START
                       1.1
#define BETA_X_END
                       0.0
#define BETA_Y_TOP
                       1.25
#define BETA_Y_BOTTOM 0.0
#define BETA Z LEFT
                       0.0
#define BETA_Z_RIGHT
                       0.0
#define TYPE of GAS
                       PERF AIR 14
```

The surface circumferential pressure distribution at x/L = 0.333 is shown in Fig. E.10. Tracy's experimental measurements [225] are also shown for comparison. Good agreement is shown between the computed solution and Tracy's data.

The experiments of Tracy [225] also included a cross-sectional Pitot survey of the flow to determine shock wave positions and the edges of boundary layers. The Pitot survey was performed along surface normals at a position 86.3 mm from the apex of the cone. A computational slice was taken in a plane perpendicular to the axis whose axial location bisects the experimental rays. The computational Mach contours on this plane are shown in Fig. E.11, along with Tracy's experimental results. Again, the computational results are in good agreement with the experimental results.



Figure E.10: Computed and experimental surface pressures around half the circumference of the cone at an axial position of x/L = 0.333.



**Figure E.11:** Computed Mach contours at x = 83 mm and Tracy's experimental flow-field Pitot survey.

# E.4 Viscous Supersonic Flow Over a Double Wedge

This test case consists of Mach 3 air flow over a corner formed by two intersecting wedges of  $9\frac{1}{2}^{\circ}$  half-angle. It was studied experimentally by West & Korkegi [235] over a range of Reynolds numbers that produced laminar, transitional and turbulent flow. The predominant flow features they observed were two wedge shocks, two embedded shocks and a corner shock. The embedded shocks interacted with the boundary layers forming on the surfaces of the wedges and caused downstream cross-flow separation. A diagram of the experiment is shown in Fig. E.12 along with a representation of the predominant flow features in a cross-stream flow plane. The laminar test flow conditions used in the experi-



Figure E.12: Experimental apparatus and cross-stream flow structure for the double wedge.

ments of West & Korkegi showed a larger cross-flow separation region than the turbulent conditions. For this reason, the laminar conditions were used for the test case. The laminar inflow conditions used were,

$$\begin{split} \rho_\infty &= 0.03634 \; \mathrm{kg/m^3}, \ u_x = 616.2 \; \mathrm{m/s}, \ u_y = u_z = 0.0 \; \mathrm{m/s}, \\ p_\infty &= 100 \; \mathrm{kPa}, \quad T_\infty = 105 \; \mathrm{K}, \quad T_{\mathrm{wall}} = 294 \; \mathrm{K}, \\ M &= 3.0 \;, \ Re_L = 2.273 \times 10^5, \end{split}$$

and the wall temperature of the wedges was 294.0 K.

The axial length of the computational domain was set to 0.0724 m which is where the experimental measurements of static wall pressure were made. The computational domain was discretized using a grid of 61 cells in both the y and z directions and 5000 cells in the axial direction. The width of each wedge was set to 0.0845 m. The parameter file and calculation macros for the wedge problem are as follows:

3D Corner	flow test c	se from West	& Korkegi 72 and Kamath 89
1004			case_id
0.4 300	0.0001		CFL, max_t_steps, tolerance
2 3 0.75			Xorder, i_supress, p_safety

```
Xi_0, dXi, X_max, max_x_steps
0.0
    0.0002 1.0 5000
0.005
                                    dXi_plot
1
                                    slice_ident
61 61
                                    nny, nnz
0 10
                                    smooth_grid, smooth_iter
      5
        5
                                    bc_N, E, S, W
3
  3
294.0 294.0 294.0 294.0
                                    Twall_N, E, S, W
0.03634 616.2 0.0 0.0 75337.5 free-stream rho, ux, uy, uz, e
0 0 0
                                    B_spline, Bezier_box, 2d format
2
                             np
0.0
         0.0
                  0.08449
                              0 A
0.0
         0.08449
                  0.08449
                               В
                               С
0.0
         0.08449
                 0.0
0.0
         0.0
                  0.0
                               D
0.07243
         0.01209
                  0.08449
                              1 A
0.07243 0.08449
                  0.08449
                               В
0.07243 0.08449
                               С
                  0.01209
0.07243 0.01209 0.01209
                               D
#define DIMENSION
                       3
#define VISC
                       1
                       0
#define TURB
#define CHEM
                       0
#define FROZEN
                       0
                       0
#define ADD HEAT
                       1
#define N_SP
#define N RE
                       1
#define BETA_X_START
                       1.2
#define BETA X END
                       0.0
#define BETA Y TOP
                       0.0
#define BETA Y BOTTOM
                       1.03
#define BETA_Z_LEFT
                       1.03
#define BETA_Z_RIGHT
                       0.0
#define TYPE_of_GAS
                       PERF_AIR_14
```

Figure E.13 shows the computed cross-stream wall pressure at an axial distance of 0.0724 m compared to the experimental results of West & Korkegi. The wall pressure shown on the vertical axis is normalized by the theoretical pressure developed behind an oblique shock generated from a two-dimensional  $9\frac{1}{2}^{\circ}$  wedge in Mach 3 flow (2168 Pa). The computed pressure asymptotes to the two-dimensional wedge pressure far from the corner, as would be expected, and the overall pressure distribution compares reasonably well with the experimental results. The computational result is very similar to other published results obtained with a PNS solver [117]. A cross-stream contour plot of density for an axial position of 0.0724 m is also shown in Fig. E.14. All the shocks associated with the three-dimensional corner flow can be clearly identified and the cross-stream separation of the boundary layer due to the adverse pressure gradient is resolved.

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Figure E.13: Cross-stream static wall pressures at an axial distance of 0.0724 m.



Figure E.14: Cross-stream density contours at an axial distance of 0.0724 m.

# E.5 Flow Through a Three-Dimensional Scramjet

A three-dimensional scramjet design with a complex internal structure was used for the fifth test case. A three-dimensional grid was generated for the internal structure using B-Spline surfaces. The scramjet module being considered for this test case was built and tested [234] in the T4 shock tunnel [207]. The module is one of six that are proposed to be placed circumferentially around a body which has a conical forebody as shown in Fig. E.15. This idea is similar to the SCRAM-MOD-1 missile design proposed by Billig [28].



**Figure E.15:** Baseline design for the scramjet-powered stage of a missile. The conical forebody and the scramjet modules are shown with the cowl removed.

The complexities of the internal surfaces are a result of the shape transitions in the inlet, combustor, and expansion nozzle. The front projection of each inlet occupies a sector of a circle, while the rear projection of each inlet is circular. The same applies for the exhaust duct but in reverse.

The surfaces required to achieve these transitions were defined as four B-Spline surfaces which were fitted using data obtained from the construction plans for the module. The B-Spline surfaces and associated control net files were generated using the software in reference [44]. The control net files were then used by sm3d to generate the computational grid as shown in Fig. E.16.

The inlet flow condition for the simulation was selected to approximate the experimental flow condition used in Wendt *et al.'s* experimental study [234]. The air test gas was assumed to be perfect with gas constants R = 287 J/kg/K and  $\gamma = 1.4$ . Gas enters



**Figure E.16:** Exterior surface of the computational grid for the three-dimensional scramjet test case constructed from B-spline surfaces. Also shown are the lines on which static pressure was measured.

the compression inlet with the following properties:

$$\label{eq:rho} \begin{split} \rho_\infty &= 0.085 \; \mathrm{kg/m^3}, \;\; u_x = 2375 \; \mathrm{m/s}, \;\; u_y = 0.0 \; \mathrm{m/s}, \;\; u_z = 0.0 \; \mathrm{m/s}, \\ p_\infty &= 10.0 \; \mathrm{kPa}, \quad T_\infty = 410 \; \mathrm{K}, \; \mathrm{and} \;\; M = 5.85 \; . \end{split}$$

The flow enters the inlet at an angle of  $0.5^{\circ}$  to the leading edge surface such that a weak shock forms. Energy was uniformly added to a block of cells to simulate hydrogen combustion by adding energy to the flow through an energy source term in the governing equations (see Eq. 2.5). The location of the heating zone was centred on x = 0.325 m with a half-length of 0.025 m. Within this heating zone, 0.9 MJ/s was added to the flow giving an effective equivalence ratio of 0.43 for an effective fuel heating value of 80 MJ/kg for gaseous hydrogen. This heating value was obtained from Fig. 6-4-2 in reference [17] assuming an average combustor temperature of 1800 K.

The input parameter file and macros used are as follows:

Compo	osite	Scramjet	Module	with	B-spline	surface,	heat a	added
1005					case_	_id		
0.1	200	0.0001			CFL,	max_t_ste	eps, to	olerance
230	.75				Xorde	er, i_supi	ress, p	safety
0.0	0.002	1.0 50	0		Xi_0,	dXi, Xi_	_max, m	nax_x_steps
0.005	5				dXi_p	olot		
1					slice	e_ident		
20 2	20				nny,	nnz		
1 1	.0				smoot	h_grid, s	smooth_	_iter

```
3 3 3 3
                                    bc_N, E, S, W
296.0 296.0 296.0 296.0
                                    Twall_N, E, S, W
                                     free_stream rho, ux, uy, uz, e
0.0850 2480.0 318.5 0.0 2.942e5
1 0 0
                                     use_B_spline, Bezier_box, 2d format
                        3
#define DIMENSION
                        0
#define VISC
#define TURB
                        0
#define CMUTM
                        0
#define CHEM
                        0
                        0
#define FROZEN
#define ADD HEAT
                        1
#define N SP
                        1
#define N RE
                        1
#define BETA_X_START
                        0.0
#define BETA_X_END
                        0.0
#define BETA_Y_TOP
                        0.0
#define BETA_Y_BOTTOM
                        0.0
#define BETA_Z_LEFT
                        0.0
#define BETA_Z_RIGHT
                        0.0
#define TYPE_of_GAS
                        PERF_AIR_14
```

Figure E.17 shows a comparison of the simulated and measured wall pressures within the scramjet module with heat addition. The set of experimental data is for a nominal fuel equivalence ratio of approximately 0.5. Despite a number of differences in detail, the comparison between the experimental data of Wendt *et al.* [234] and the computed



**Figure E.17:** Comparison of simulated and measured wall pressures within the scramjet module with heat addition. The symbols denote measured pressures and the lines represent the computational pressures along the lines indicated in Fig. E.16.

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pressure levels is reasonable. Viscous and turbulence effects were not included in the simulations. These effects can be expected to influence the data toward the end of the compression inlet ( $x \simeq 0.2$  m), within the combustor, and near the beginning of the thrust nozzle ( $x \simeq 0.75$  m).

### E.6 Hydrogen Combustion in a Scramjet Combustor

Supersonic hydrogen/air ignition and combustion in a constant area duct was used as the sixth test case for the finite-rate chemistry functions implemented within sm3d. The test conditions were taken from the manual for the chemical kinetics code, NASAC, written by Bittker and Scullin [29]. The NASAC code is a fully implicit code that uses set values for heats of reactions, rather than using formation enthalpies to determine the energy released or consumed in a particular reaction (as is the case in sm3d).

The air and hydrogen were assumed to be perfectly mixed in a stoichiometric ratio of 1. The initial conditions of the mixture entering the duct were,

$$\label{eq:rho} \begin{split} \rho &= 0.15628 \; \mathrm{kg/m^3}, \; u = 4551.7 \; \mathrm{m/s}, \; e = 1.711 \times 10^6 \; \mathrm{J/kg}, \\ p &= 0.9686 \times 10^6 \; \mathrm{Pa}, \; T = 1559 \mathrm{K} \; \mathrm{and} \; M = 5.04 \; \; . \end{split}$$

The ignition and combustion process was modelled with 15 possible reaction paths and 9 species [29] (see Table C.3). A computational domain of 4000 axial cells, with a minimum of 2 cells in both the  $\eta$  and  $\zeta$  directions was used as an approximation of a one-dimensional flow domain. The cells were spread out over 760 mm to capture the entire combustion process up to its equilibrium state.

The parameter file and macros used for this test case were,

```
Hydrogen combustion in a constant area duct
1006
                             case_id
0.1 300 0.0001
                             CFL, max_t_steps, tolerance
2 1 1.0
                             Xorder, i_supress, p_safety
0.0 0.00025 1.0 4000
                             Xi_0, dXi, X_max, max_x_steps
0.002
                             dXi_plot
1
                             slice_ident
2 2
                             nny, nnz
0 0
                             smooth grid, smooth iter
        3
3 3 3
                             bc N, E, S, W
297.0 297.0 297.0 297.0
                             Twall N, E, S, W
1.56283e-1 4551.73 0.0 0.0 1.711086e6 free-stream rho, ux, uy, uz, e
0 0 1
                             use_B_spline, Bezier_box, 2d format
2
                             np
0.0 0.0
                             0 A
0.0 2.0
                               В
0.76 0.0
                             1 A
0.76 2.0
                               В
```

#define	DIMENSION	2
#define	VISC	0
#define	TURB	0
#define	CMUTM	0
#define	CHEM	1
#define	FROZEN	0
#define	ADD_HEAT	0
#define	N_SP	9
#define	N_RE	15
#define	BETA_X_START	0.0
#define	BETA_X_END	0.0
#define	BETA_Y_TOP	0.0
#define	BETA_Y_BOTTOM	0.0
#define	BETA_Z_LEFT	0.0
#define	BETA_Z_RIGHT	0.0
#define	TYPE_of_GAS	NON_EQ

The steady state species mass fractions calculated using sm3d and NASAC are shown in Fig. E.18. The figure shows a good comparison between the solutions of the two



**Figure E.18:** Species mass fractions along a constant area duct resulting from hydrogen combustion in air. The lines represent the results obtained from *sm3d*, and the symbols represent results from NASAC [29].

codes. The calculated steady state flow variables at the end of the duct are given in Table E.1 alongside the inflow conditions for comparison.

	Inflow Conditions	Steady State Exit Condition	
		NASAC	sm3d
u, (m/s)	4551.7	4440.8	4441.6
$ ho, \ \mathrm{kg/m^3}$	0.15628	0.16018	0.16012
p, kPa	96.8	175.7	175.5
Т, К	1559	3016	3015
М	5.04	3.78	3.79

**Table E.1:** Inflow and exit, steady state flow variables for the hydrogen combustion test case presented in the NASAC manual [29].

### E.7 Turbulent Two-Dimensional Flow over a Flap

The seventh test case is from the hypersonic, turbulent boundary layer experiments performed by Coleman & Stollery [42] and was used to test the solver's implementation of the Baldwin & Lomax turbulence model [20]. The experiment consisted of a sharp flat plate with a trailing edge flap as shown in Fig. E.19. The trailing edge flap was hinged



Figure E.19: Two-dimensional flat plate and flap used for hypersonic turbulent flow experiments of Coleman & Stollery [42].

so that several corner angles could be studied. The experimental results for a flap angle of  $30^{\circ}$  were used for the current test case because it was the largest angle that could be set before the flow separated. The test gas was low temperature air issuing from a hypersonic gun tunnel. The simulated inflow conditions were,

$$\begin{split} \rho_{\infty} &= 0.15094 \; \text{kg/m^3}, \;\; u_x = 1424.87 \; \text{m/s}, \;\; u_y = 0.0 \; \text{m/s}, \;\; u_z = 0.0 \; \text{m/s}, \\ p_{\infty} &= 2.608 \; \text{kPa}, \quad T_{\infty} = 59.4 \; \text{K}, \quad T_{\text{wall}} = 295 \; \text{K}, \\ M &= 9.22 \;, \;\; \text{and} \;\; Re_L = 3.06 \times 10^7. \end{split}$$

The computations were performed assuming a turbulent boundary layer from the leading edge of the plate to the end of the trailing edge flap. The wall temperature was set at a constant 295 K. Due to the strong interaction of the developed boundary layer and the shock emanating from the flap, the computations were performed in stages using two grids. The first grid was used to simulate the growth of turbulent boundary layer along the flat plate up to the flap. The second grid was used to simulate the flow over the trailing edge flap. A larger number of axial cells were used for the flap grid to maintain the stability of the computations. The two grids are shown in Fig. E.20. A clustering parameter



**Figure E.20:** Two-dimensional grids used for the hypersonic turbulent two-dimensional flow over a flap test case (grid formed from cell centres).

of 1.001 was used for cells next to the wall in both grids. This strong clustering ensured that the  $y^+$  value of the cells nearest to the wall remained less than 7.3.

The parameter files and macro settings used for this test case are,

```
Turbulent Hypersonic Boundary flow over a 30 deg Flap - str
1007
                              case_id
0.4 400 0.0001
                              CFL, max_t_steps, tolerance
2 5 0.75
                              Xorder, i_supress, p_safety
0.0 0.0001 1.0 10000
                              Xi O, dXi, X max, max x steps
0.005
                              dXi plot
                              slice_ident
1
60
    2
                               nny, nnz
0 0
                              smooth_grid, smooth_iter
                              bc_N, E, S, W
1
   3 5 3
295.0 295.0 295.0 295.0
                              Twall N, E, S, W
0.1529 1424.9 0.0 0.0 42648.2 free-stream rho, ux, uy, uz, e
0 0 1
                              use_B_spline, Bezier_box, 2d format
2
                              np
-0.56 0.0
                              0 A
-0.56 0.03
                                В
0.0
      0.00
                              1 A
0.0
      0.08
                                В
#define DIMENSION
                        2
                        1
#define VISC
#define TURB
                        1
                        0
#define CMUTM
                        0
#define CHEM
#define FROZEN
                        0
#define ADD_HEAT
                        0
#define N_SP
                        1
#define N RE
                        1
#define BETA_X_START
                        1.1
#define BETA_X_END
                        0.0
#define BETA_Y_TOP
                        0.0
#define BETA_Y_BOTTOM
                        1.001
```

#define BETA Z LEFT 0.0 #define BETA\_Z\_RIGHT 0.0 #define TYPE\_of\_GAS PERF\_AIR\_14 \_\_\_\_\_ Turb. Hypersonic Boundary flow over a 30 deg Flap - ramp section 1007 case\_id 0.25 2000 0.0001 2 5 0.75 CFL, max\_t\_steps, closing tolerance 2 5 0.75 Xorder, i\_supress, p\_safety 0.0 0.00001 1.0 100000 Xi\_0, dXi, X\_max, max\_x\_steps 0.005 dXi\_plot slice ident 1 60 2 nny, nnz smooth\_grid, smooth\_iter 0 10 1 3 5 3 bc\_N, E, S, W 295.0 295.0 295.0 295.0 Twall\_N, E, S, W 0.1529 1424.9 0.0 0.0 42648.2 free-stream rho, ux, uy, uz, e 0 0 1 use\_B\_spline, Bezier\_box, 2d format 2 np 0.0 0.00 0 A 0.0 0.08 В 0.075 0.0433 1 A 0.075 0.0933 В #define DIMENSION 2 #define VISC 1 #define TURB 1 #define CMUTM 0 #define CHEM 0 #define FROZEN 0 #define ADD\_HEAT 0 #define N\_SP 1 #define N\_RE 1 #define BETA\_X\_START 0.0 #define BETA\_X\_END 0.0 #define BETA\_Y\_TOP 0.0 #define BETA\_Y\_BOTTOM 1.001 #define BETA\_Z\_LEFT 0.0 #define BETA\_Z\_RIGHT 0.0 #define TYPE\_of\_GAS PERF\_AIR\_14

Figure E.21 compares the experimentally measured and simulated pressure and heat transfer coefficients along the surface of the plate and flap. The surface heat transfer coefficient is non-dimensionalized by the coefficient value at a point just upstream of the corner. The pressure coefficient is also non-dimensionalized by the value just upstream of the corner. The coefficient of pressure is defined by the expression,

$$C_p = \frac{p}{\rho_\infty u_\infty^2} \quad ,$$

and the heat transfer coefficient is defined by the same expression used for the compression corner case (Eq. E.1). The calculated pressure coefficients on the flap show reasonable agreement with the experimental values, and the computational results approach the expected pressure of an inviscid solution far from the wall [231]. The computational



**Figure E.21:** Compression corner flow with  $30^{\circ}$  flap angle. The two plots show the experimental data of Coleman & Stollery [42](symbols) compared with the computational results (lines) for (a) surface pressure coefficient and (b) surface heat transfer coefficient.

heat transfer values as predicted using the Baldwin & Lomax turbulence model [20] are slightly higher than those measured in the experiment of Coleman & Stollery [42]. This is consistent with other simulations performed using the same turbulence model [95, 231] and seems to be a function of the turbulence model rather than a problem with its implementation in *sm3d*.

### E.8 Viscous Flow over a Cylinder

The implementation of the axisymmetric viscous terms was examined by computing the supersonic, viscous flow over a hollow cylinder. The flow geometry consists of a hollow cylinder aligned with the x-axis. The cylinder is 1.0 m long and has a radius of 0.005 m. A uniform Mach 2 flow of air was used as the free-stream where the uniform inflow conditions were,

$$\rho_{\infty} = 0.00404 \text{ kg/m}^3, \ u_x = 597.3 \text{ m/s}, \ u_y = 0.0 \text{ m/s}, \ u_z = 0.0 \text{ m/s},$$
  
 $p_{\infty} = 257.4 \text{ Pa}, \quad T_{\infty} = 222 \text{ K}, \quad T_{\text{wall}} = 222 \text{ K},$   
 $M = 2.0, \text{ and } Re_L = 1.7 \times 10^5.$ 

The air was assumed to be calorically perfect with  $\gamma = 1.4$ , R = 287 J/kg/K and a constant Prandtl number of 0.72. The grid was shaped to capture the leading edge incident shock (LEIS) and divided into  $2000 \times 50$  cells (see Fig. E.22).



**Figure E.22:** Computational grid joining cell centres, that was used for the viscous flow over a cylinder test case (only every tenth axial cell shown).

The South boundary, which coincides with the cylinder surface, was set to a no-slip boundary condition with a constant temperature of  $T_{\text{wall}} = 222.0$  K. The top (North) boundary was supersonic inflow, and the remaining East and West boundaries were reflective boundaries. The free-stream inflow conditions and calculation macros used are presented in the parameter file and macro listing that follows.

Viscous flow along a cylinder 1008 case\_id 0.4 400 0.0001 CFL, max\_t\_steps, tolerance

```
2 3 0.75
                             Xorder, i_supress, p_safety
0.0 0.0005 1.0 2000
                             Xi_0, dXi, X_max, max_x_steps
0.005
                             dXi_plot
1
                             slice_ident
50 2
                             nny, nnz
0 10
                             smooth_grid, smooth_iter
1 3 5 3
                             bc_N, E, S, W
222.0 222.0 222.0 222.0
                             Twall_N, E, S, W
0.00404 597.3 0.0 0.0 1.59285e5 free-stream rho, ux, uy, uz, e
0 0 1
                             use_B_spline, Bezier_box, 2d
2
                             np
0.0
    0.005
                             0 A
0.0 0.065
                               В
1.0 0.005
                             1 A
1.0 0.705
                               В
#define DIMENSION
                       0
#define VISC
                       1
#define TURB
                       0
#define CMUTM
                       0
                       0
#define CHEM
                       0
#define FROZEN
#define ADD_HEAT
                       0
#define N_SP
                       1
#define N_RE
                       1
#define BETA_X_START
                       1.04
#define BETA_X_END
                       0.0
#define BETA_Y_TOP
                       0.0
#define BETA Y BOTTOM 1.004
#define BETA_Z_LEFT
                       0.0
#define BETA_Z_RIGHT
                       0.0
#define TYPE_of_GAS
                       PERF_AIR_14
```

The pressure contour plot of the solution in Fig. E.23 shows the development of a weak leading edge interaction shock (LEIS). Figure E.24 compares the computed x-velocity and temperature profiles through the boundary layer at an axial location of x = 0.916 m, with the profiles computed by a highly accurate boundary layer algorithm which is based on a spectral collocation method [172]. The agreement is very good with a maximum variation in axial velocity of 1.4%.

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Figure E.23: Pressure contours for the axisymmetric flow over a cylinder.



**Figure E.24:** The cross-stream (a) x-velocity profile and (b) temperature profile at an axial location of x = 0.916 m. The *sm3d* solution is shown as symbols and a spectral solution [172] is shown as solid lines.

# E.9 Test Case Computation Times

All of the test cases were run in serial on The University of Queensland's Silicon Graphics Origin 2000 (see Appendix G). At the time of writing this study, the machine was equipped with 64 model R10000 processors, although only one processor was used to perform each test case. The speed of the solver running on this machine was calculated for each case by dividing the computational time (or CPU time) by the number of cells in the cross-stream and total number of iterations in time for each cross-stream slice. The solver speed for each case is listed in Table E.2, and the solver configuration for each case is summarised in Table E.3. The solver speed for the 3-D Scramjet case shows that a large

Case name	Mesh size			CPU time	Solver speed
				(sec)	( $\mu$ s/cell/step)
Flat Plate	1000	$\times 100$		708	46.7
Compression Corner	2000	$\times$ 90		2096	42.2
Cone at Angle of Attack	1000	$\times$ 50	$\times$ 56	771780	46.0
Double Wedge	5000	× 61	× 61	29118	50.1
3-D Scramjet	500	imes 20	imes 20	177	21.9
Hydrogen Combustion	8000	$\times 2$		594	59.4
Turbulent Flap - plate	10000	$\times$ 60		3365	47.6
Turbulent Flap - flap	100000	$\times$ 60		11379	51.0
Viscous Cylinder	2000	$\times$ 50		186	40.0

Table E.2: Computation times and speeds for all of the test cases.

Table E.3: Configuration of the solver when used to perform the test cases.

Case name	Viscous	Turbulence	Finite-rate	Axisymmetric
	terms	model	chemistry	terms
Flat Plate				
Compression Corner				
Cone at Angle of Attack				
Double Wedge				
3-D Scramjet				
Hydrogen Combustion			$\checkmark$	
Turbulent Flap - plate		$\checkmark$		
Turbulent Flap - flap				
Viscous Cylinder				$\checkmark$

increase in solver speed results when the viscous terms are dropped from the governing equations. However, the solver speed for the hydrogen combustion case demonstrates that this speed is lost when a complex finite-rate reaction model is introduced into the equation set. Overall, the results show that the solver speed is predominantly dependent on the complexity of the models and equations used in the flow solver for a particular problem.
## **Parameter File**

The parameter file is the primary data file that defines the computational problem to be solved by the flow solver. This appendix presents a line by line description of the contents of a parameter file. Examples of parameter files for a set of test case problems are given in Appendix E.

The format of the parameter file is specified using the C-language notation. A "%f" indicates that a floating-point number is expected, while "%d" indicates an integer, and "%s" indicates a string of characters.

line 1 %s : title string of up to 132 characters

line 2 %d : *case\_id*, primarily used for custom geometry routines and optimization problems.

line 3 %f %d %f : CFL, max\_t\_steps, tolerance

- The *CFL* number is a stability factor that should always be less than 0.5 (see Section 2.13).
- max\_t\_steps is the limit on the number of time steps permissible for any slice of cells to reach a steady state. If this limit reached, the calculation algorithm moves to the next downwind slice. Typically max\_t\_steps is set to 200 for nonreacting flows and 500 for reacting flows.
- tolerance specifies the cell density steady state tolerance. A change in cell density less than tolerance between time steps indicates that a steady state has been achieved in that cell. Typically this value is set to  $10^{-4}$ . As a consistency check, tolerance should be decreased by an order of magnitude to see if the solution at each slice has reached a genuine steady state.

line 4 %d %d %f : Xorder, i\_suppress, p\_safety

- *Xorder* specifies the order of reconstruction. A value of 1 sets low-order reconstruction (i.e. none) and a value of 2 sets high-order reconstruction.
- *i\_suppress* indicates the number of streamwise slices from the initial slice, where the pressure gradient is set to 0 in the boundary layer to maintain stability (recommended value is 3). Used for viscous flow only.
- *p\_safety* is the safety factor which maintains real positive eigenvalues in the boundary layer. It is typically set between 0.75 (high viscous interactions) and 1.0 (low interactions). Used for viscous flow only (see Section 2.5).

- line 5 %f %f %f %d : Xi, dXi, Xi\_max, max\_x\_steps
  - $Xi(=\xi)$  is the starting point for the calculation in normalized (computational) coordinates  $0 \le \xi \le 1.0$ .
  - dXi: streamwise step size. This should be selected to ensure that the cells do not become too elongated.
  - Xi\_max: a downstream limit for the calculation
  - *max\_x\_steps*: a limit on the number of space-marching steps
- line 6 %f : *dXi\_plot* 
  - *dXi\_plot* is the normalized distance between slices that are written to the output file. The data in the output file can then be picked up by the post-processing programs and used for plotting.
- line 7 %d : ident
  - *ident* is a domain block identifier that is intended for use in the future multi-flow-path version of the code.
- line 8 %d %d : *nny*, *nnz* 
  - *nnz* and *nny* are the numbers of cells in the  $\zeta$  and  $\eta$  directions respectively.
- line 9 %d %d : *smooth\_grid*, *smooth\_iter* 
  - *smooth\_grid* is a switch for a Laplacian grid smoother. The grid smoother essentially averages neighbouring points to get the new coordinates of the point.
  - *smooth\_iter* is used to set the number of Laplacian iterations.
- line 10 %d %d %d %d : *bc\_N*, *bc\_E*, *bc\_S*, *bc\_W* 
  - These integers set the wall boundary-condition and may take the following values:
    - 0 : adjacent to another flow path
    - 1 : supersonic inflow condition
    - 2 : supersonic outflow (not used)
    - 3 : solid wall with inviscid (slip) tangency condition
    - 4 : solid, no-slip, adiabatic wall
    - 5 : solid, no-slip, fixed temperature wall

line 11 %f %f %f %f : Twall\_N, Twall\_E, Twall\_S, Twall\_W

- Wall temperatures for viscous flows.

line 12 %f %f %f %f %f %f ;  $\rho$ ,  $u_x$ ,  $u_y$ ,  $u_z$ , e

- These are the free-stream flow conditions.

 $\rho$  : density in kg/m<sup>3</sup>  $u_x, u_y, u_z$  : velocity components in m/s e : specific internal energy in J/kg

line 13 %d %d : use\_B\_splines, use\_bezier\_box, 2d

- use\_B\_splines is set to 1 to use the data from the control net files < bfn > .q1, q2, q3, q4 to create the grid.

- use\_bezier\_box is set to 1 to use the point coordinates on the following lines as control points for bezier curves that define the streamwise edges of the grid domain.
- -2d is set to 1 for two dimensional flow cases so that the code automatically sets the *z* coordinates of the three-dimensional grid.
- If both set *use\_B\_splines* and *use\_bezier\_box* are set to 0 and there are no hard coded geometries for the case being considered, the grid will be made up of quadrilateral panels between the cross-sections that follow.

For cases where the grid is "hard-coded", the remaining lines are not necessary in the input file.

line 14 %d : *np* 

- np is the number of quadrilateral cross-sections used to define the duct. Each cross-section is defined by its corner points in 3-D space. If the 2d switch is set, only two points need to be specified in x, y space.
- line 15 %f %f %f : PA.x, PA.y, PA.z are the coordinates for point A in m.

line 16 %f %f %f : *PB.x, PB.y, PB.z* are the coordinates for point B in m.

line 17 %f %f %f : *PC.x*, *PC.y*, *PC.z* are the coordinates for point C in m.

line 18 %f %f %f : *PD.x*, *PD.y*, *PD.z* are the coordinates for point D in m.

Note that lines 15 to 18 are repeated for each *ip* cross-section  $0 \le ip < np$ .

# SGI Origin 2000

All of the flow simulations presented in this thesis and the majority of the code development for *sm3d* were conducted on The University of Queensland's Silicon Graphics Origin 2000 system (shown in Fig. G.1) running IRIX Release 6.4. The Origin 2000 at



Figure G.1: The Silicon Graphics Origin 2000 Rack.

The University of Queensland is a shared memory multiprocessor system with processors and memory linked by a high speed switch interconnect. The Origin 2000 is currently configured with 64 MIPS R10000 CPUs and 16 G bytes of memory. Disks attached to the system provide 40 G byte of Raid5 for users home directorys plus 100 G byte of high speed filesystems for applications and working space. Technical information relating to the processors and node cards is presented in Table G.1. Additional technical information can be obtained from the SGI world wide web site: www.sgi.com/origin/2000\_specs.html

	Processor Data		
Microprocessor	MIPS RISC R10000 64-bit CPU		
Primary caches	32KB two-way set-associative on-chip instruction cache		
	32KB two-way set-associative on-chip data cache		
Secondary cache	e 4MB two-way set-associative cache per CPU		
	Node Card		
CPU capacity	2 R10000 CPUs		
Memory	512MB ECC protection capacity SDRAM		
HW cache coherency	yes		
Interleaving	32-way per node card		
Memory	680MB/sec sustained		
bandwidth	780MB/sec peak		

Table G.1: Detailed specifications of the Origin 2000 rack at the University of Queensalnd.

# Mach 7 Nozzle Technical Drawings

Sheet	Item
1	Subsonic Contraction - Dimensions
2	Subsonic Contraction - Bezier Control Points
3	Initial Expansion Insert - Dimensions
4	Initial Expansion Insert - Bezier Control Points
5	Contoured Nozzle Block - Dimensions
6	Contoured Nozzle Block - Bezier Control Points
7	Throat Shell - Dimensions
8	End Cover - Dimensions

















# **Pressure Transducers and Calibration Results**

### Contents

- Operating guide and specifications for the PCB piezoelectric pressure transducers
- Calibration curves for transducers 14534, 14535 and 14536
- Calibration curve for the supply cylinder pressure gauge





MODEL 102A02, 102A05, 102A07, 112A21, 112A22, 112A23 OPERATING GUIDE

## REVISIONS ECR # 2803 SHEET 2 OF 3

#### 3.0 INSTALLATION (con't)

the factory. Replace seals when they become unserviceable.

In some cases, e.g., where flash temperatures such as those generated by combustion processes are present, it may be necessary to thermally insulate the diaphragm to minimize spurious signals generated by these effects.

Common black vinyl electrical tape has been found to be an effective insulating material in many cases. One or more layers may be used, across the end of the diaphragm without affecting response or sensitivity.

A silicone rubber coating approximately .010" thick has also been proven effective in many applications. GE type 560 silicone rubber kit with SS4004 primer is recommended. First treat the surface with the primer, then apply the rubber coating and allow to cure in accordance with the manufacturer's instructions.

Although ICP transducers have low output impedance and in general are not affected by moisture, in extreme environments it is good practice to protect cable connections with shrink tubing.

It is not necessary to use low noise coaxial cable with this transducer series, in fact a Model 070A09 solder connector adaptor allows the use of ordinary 2-wire cable is desired.

#### 4.0 OPERATION

It is only necessary to supply the transducer with a 2-20 mA constant current at +18 to +24 VDC through a current regulating diode or equivalent circuit. (See Guide G0001 for powering and signal utilization information pertaining to all ICP instrumentation). Most of the power units manufactured by PCB has an adjustable current feature allowing a choice of input currents from 2 to 20 mA. In general, for lowest noise (best resolution) choose the low current ranges and for driving long cables (to several thousand feet) use the higher current, up to 20 mA maximum.

To operate system using a PCB power unit:

Switch power on.

2. Wait several minutes for the IC amplifier to turn on and stabilize and if AC coupled to readout instrument (as with 482A and 483A Series Power Units and with 485A and B Power Conditioners) wait five times the coupling time constant for coupling capacitor to fully charge.

3. Proceed with measurements.

#### 4.1 OPERATING CONSIDERATIONS FOR

MODEL 112A23

The Model 112A23 features a low noise amplifier which, based on a peak-to-peak broadband noise factor of 50 µV, results in a resolution of .001 psi.

Defined for practical purposes as the minimum readout signal, the resolution is based on the sensitivity of 50 mV/psi and a low noise amplifier of 50 uV peak noise.

Thus,  $\frac{50 \text{ uV}}{50 \text{ mV}}$  = .001 psi resolution

The output bias voltage of the Model 112A23 is 5.0 volts, half the bias voltge of most PCB pressure transducers. This will cause the bias monitor meter on PCB power supplies to read at the low end of the green band.

### **Pressure Transducers and Calibration Results**

PCB	OPERATING GUIDE		REVISIONS ECR # 2803		
Piccornonios			3 OF 3		
5.0 POLARIT	<u>ry</u>	8.0 MAINTENANCE			
This transducer series produces a positive-going output voltage for increasing pressure input.		The miniature size sealed construction precludes field maintenance. Should service be required, return unit to			
6.0 LOW FRE	QUENCY RESPONSE	factory with note describing problem.			
The low fre system is d	equency response of an ICP determined by:				
<ol> <li>The dis transducer,</li> </ol>	charge time constant of the and,				
<ol> <li>If AC c coupling ti</li> </ol>	poupled at power unit, the me constant.				
Consult Sec G0001 for d frequency c ments.	tions 6.0 through 6.2 in Guide etailed explanation of low haracteristics of ICP instru-				
7.0 CALIBRA	TION				
Piezoelectr devices but may be empl. stants are static meth several hum constant.	ic transducers are dynamic static calibration methods oyed if discharge time con- sufficiently long. Generally, ods are not employed below dred seconds discharge time				
To employ s the transduc T-connector Model 4848 Apply press and take rea sure after o	tatic methods, direct couple cer to the DVM readout using a from the XDCR jack or use the in the "calibrate" mode. ure with dead weight tester adings quickly. Release pres- each calibration point.				
For the show series, a ra	rter discharge time constant apid pressure step must be				

generated by a pneumatic pressure pulse calibrator or dead weight tester and readout is by recorder or storage oscilloscope.

PCB offers a complete recalibration service. Consult factory for details.

### Pressure Transducers and Calibration Results

	<b>PFR</b> SF	SPECIFICATIONS		-D- REV #2366		
	Рискотволісь Р	VOLTAGI RESSURE T	E OUTPUT RANSDUCER		SHEET OF 1	
	MODEL NO		112A21	112A22	112A23	
	RANGE (V) OUTPUT	psi	100 (5)	50 (5)	50 (2.5)	
	USEFUL OVERRANGE	psi	200	50	50	
	MAXIMUM PRESSURE	psi	1000	1000	1000	
	RESOLUTION	psi	.002	.001	.001	
	SENSITIVITY	mV/psi	50 <sup>+</sup> 10	100	50 <sup>+</sup> 10	
	RESONANT FREQUENCY	kHz	250	250	260	
	RISE TIME	µSec	2	2	200	
	DISCHARGE TIME CONST	Sec	>1	> 1	>1	
	LOW FREQ RESPONSE-5%	Hz	.50	.50	50	
	LINEARITY A	% FS	1	1	1	
	POLARITY		POSITIVE	POSITIVE	POSITIVE	
	OUTPUT IMPEDANCE	ohm	<100	<100	<100	
	OUTPUT BIAS +	volt	8 to 14	8 to 13.5	3 to 8	
	OVERLOAD RECOVERY	µSec	10	10	10	
	ACCELERATION SENS TEMP COEFFICIENT TEMPERATURE RANGE MAXIMUM FLASH TEMP VIBRATION/SHOCK	psi/G %/ <sup>O</sup> F OF OF G's peak	.002 ≤.03 -100 to +275 3000 2000/20000	.002 ≤.03 -100 to +27 3000 2000/20000	.002 ≤.03 5 -100 to +275 3000 2000/20000	
	SEALING CASE/DIAPHRAGM MAT'L WEIGHT w/CLAMP NUT CONNECTOR (micro)	gm coaxial	EPOXY 17-4/INVAR 6 10-32	EPOXY 17-4/INVAR 6 10-32	EPOXY 17-4/INVAR 6 10-32	
	EXCITATION	+VDC/mA	24-27/2-20	24-27/2-20	10-28/2-20	
AT ROOM TEMPERATURE						
1	▲ ZERO BASED BEST STRA	IGHT LINE.				
	SUPPLIED ACCESSORIES: SEAL MOD. 065A02 CLAMP NUT MOD. 060A03		APP'D The ENGR Muto SALES · RCM	12/22 SPEC No. 12, 374 112 12/82	-1210-80	



Figure I.1: Calibration results for Pitot #1 : Transducer serial No. 14534. Model number 112A21.



Figure I.2: Calibration results for Pitot #2 : Transducer serial No. 14535. Model No. 112A21.



Figure I.3: Calibration results for Pitot #3 : Transducer serial No. 14536. Model No. 112A21.



Pressure Gauge Calibration

Figure I.4: Calibration results for the gas cylinder pressure gauge.

## **Bibliography**

- Abgrall, R., Fezoui, L., and Talandier, J., "An Extension of Osher's Riemann Solver for Chemical and Vibrational Nonequilibrium Gas Flows," *Int. J. for Numerical Methods in Fluids*, Vol. 14, 1992, pp. 935–960.
- [2] Alcenius, T., Schneider, P., Beckwith, I. E., White, J. A., and Korte, J. J., "Development of Square Nozzles for Supersonic Low-Disturbance Wind Tunnels," AIAA Paper 94-2578, June 1994.
- [3] Alcenius, T., Schneider, P., Beckwith, I. E., White, J. A., and Korte, J. J., "Development of Square Nozzles for Supersonic Low-disturbance Wind Tunnels," *Journal* of Aircraft, Vol. 33, No. 6, 1996, pp. 1131–1138.
- [4] Amann, H. O., "Experimental Study of the Starting Process in a Reflection Nozzle." *The Physics of Fluids Supplement*, Vol. I, 1969, pp. I–150–I–153.
- [5] Anderson, D. A., Tannehill, J. C., and Pletcher, R. H., *Computational Fluid Me-chanics and Heat Transfer*, Hemisphere Publishing Corporation, New York, 1984, pp. 431–432.
- [6] Anderson, G. Y., Kumar, A., and Erdos, J., "Progress in Hypersonic Combustion Technology with Computation and Experiment," AIAA Paper 90-5254, Oct 1990.
- [7] Anderson, J. D., *Hypersonic and High Temperature Gas Dynamics*, McGraw-Hill, New York, 1989, pp. 379.
- [8] Anderson, J. D., *Hypersonic and High Temperature Gas Dynamics*, McGraw-Hill, New York, 1989, pp. 453.
- [9] Anderson, J. D., *Hypersonic and High Temperature Gas Dynamics*, McGraw-Hill, New York, 1989, pp. 439.
- [10] Anderson, J. D., Hypersonic and High Temperature Gas Dynamics, McGraw-Hill, New York, 1989, pp. 54.
- [11] Anderson, J. D., Modern Compressible Flow: with Historical Perspective. 2nd Edition, McGraw-Hill, New York, 1990, pp. 327.

- [12] Anderson, J. D., Modern Compressible Flow: with Historical Perspective. 2nd Edition, McGraw-Hill, New York, 1990, pp. 18.
- [13] Anderson, J. D., *Modern Compressible Flow: with Historical Perspective. 2nd Edition*, McGraw-Hill, New York, 1990, pp. 329.
- [14] Anderson, J. D., Modern Compressible Flow: with Historical Perspective. 2nd Edition, McGraw-Hill, New York, 1990, pp. 327.
- [15] Anderson, J. D., Modern Compressible Flow: with Historical Perspective. 2nd Edition, McGraw-Hill, New York, 1990, pp. 325.
- [16] Anderson, W. K., Thomas, J. L., and van Leer, B., "A Comparison of Finite Volume Flux Vector Splittings for the Euler Equations," AIAA Paper 85-0122, 1985.
- [17] Archer, R.D. Saarlas, M., Introduction to Aerospace Propulsion, Prentice-Hall, Upper Saddle River, N.J., 1996.
- [18] Austin, J. M., Jacobs, P. A., Kong, M. C., Barker, P., Littleton, B. N., and Gammie, R., "The Small Shock Tunnel Facility at UQ," Department of Mechanical Engineering Report 2/97, University of Queensland, 1997.
- [19] Bakos, R. and Erdos, J., "Optimizing Pressure Recovery in a Detonation Driven Reflected Shock Tunnel," *Proceedings 21th International Symposium on Shock Waves*, July 20-25 1997, pp. 1359–1365.
- [20] Baldwin, B. S. and Lomax, H., "Thin Layer Approximation and Algebraic Model for Separated Turbulent Flows," AIAA Paper 78-257, Jan. 1978.
- [21] Baulch, D. L., Drysdale, D. D., Horne, D. G., and Lloyd, A., Evaluated Kinetic Data for High Temperature Reactions. Volume 1-Homogeneous Gas Phase Reactions of the H2-O2 System, CRC Press, New York, 1972.
- [22] Baysal, O. and Eleshaky, M., "Aerodynamic Design Optimization Using Sensitivity Analysis and Computational Fluid Dynamics," *AIAA Journal*, Vol. 30, No. 3, 1992, pp. 718–725.
- [23] Baysal, O., Eleshaky, M., and Burgreen, G., "Aerodynamic Shape Optimization Using Sensitivity Analysis on Third-Order Euler Equations," *Journal of Aircraft*, Vol. 30, No. 6, 1993, pp. 953–961.
- [24] Beckwith, I. E., Ridyard, H. W., and Croner, N., "The Aerodynamic Design of High Mach Number Nozzles Utilizing Axisymmetric Flow with Application to a Nozzle of Square Section," NACA TN 2711, 1952.

- [25] Benton, J., Perkins, J., and Edwards, A., "Limitations of the Methods of Characteristics When Applied to Axisymmetric Hypersonic Nozzle Design," AIAA Paper 90-0192, Jan. 1990.
- [26] Bhutta, B. and Lewis, C., "Prediction of Three-Dimensional Hypersonic Reentry Flows using a PNS Scheme," AIAA Paper 85-1604, 1985.
- [27] Billig, F. S., "Research on Supersonic Combustion," Journal of Propulsion and Power, Vol. 9, No. 4, 1993, pp. 499–514.
- [28] Billig, F. S., "SCRAM-A Supersonic Combustion Ramjet Missile," AIAA Paper 93-2329, 1993.
- [29] Bittker, D. A. and Scullin, V. J., "General Chemical Kinetics Computer Program for Static and Flow Reactions, with Application to Combustion and Shock-Tube Kinetics," NASP Technical Memorandum TND-6586, 1972.
- [30] Boyton, F. P. and Thomson, A., "Numerical Computation of Steady, Supersonic, Two-Dimensional Gas Flow in Natural Coordinates," *Journal of Computational Physics*, Vol. 3, 1969, pp. 379–398.
- [31] Bradshaw, B., *Experimental Fluid Mechanics*, Pergamon Press, Oxford, 1970.
- [32] Broadbent, E. G., "Flows with Heat Addition," *Progress in Aerospace Science*, Vol. 17, No. 2, 1976, pp. 93–108.
- [33] Buggeln, R., MacDonald, H., Kreskovsky, J., and Levy, R., "Computation of Three-Dimensional Viscous Supersonic Flows in Inlets," AIAA Paper 80-0194, 1980.
- [34] Burgreen, G. W., Baysal, O., and Eleshaky, M. E., "Improving the Efficiency of Aerodynamic Shape Optimization," *AIAA Journal*, Vol. 32, No. 1, 1994, pp. 69– 76.
- [35] Candler, G. and MacCormack, R., "The Computation of Hypersonic Ionized Flows in Chemical and Thermal Nonequilibrium," AIAA Paper 88-0511, Jan. 1988.
- [36] Candler, G. and Perkins, J., "Effects of Vibrational Nonequilibrium on Axisymmetric Hypersonic Nozzle Design," AIAA Paper 91-0297, Jan. 1991.
- [37] Cebeci, T. and Smith, A., Analysis of Turbulent Boundary Layers., Academic Press, New York, 1974.
- [38] Chakravarthy, S. R., "Development of Upwind Schemes for the Euler Equations," NASA Contractor Report 4043, 1987.

- [39] Chang, C. L., Kronzon, Y., and Merkle, C. L., "Time-Iterative Solutions of Viscous Supersonic Nozzle Flows," *AIAA Journal*, Vol. 26, No. 10, 1988, pp. 1208–1215.
- [40] Chapman, S. and Cowling, T. G., *The Mathematical Theory of Nonuniform Gases*, *3rd Edition*, Cambridge University Press, London, 1970.
- [41] Chase, M. W., JANAF Thermochemical Tables, American Institute of Physics, New York, N.Y., 1985.
- [42] Coleman, G. T. and Stollery, J. L., "Heat Transfer in Hypersonic Turbulent Separated Flow," Report 72-05, Department of Aeronautics, Imperial College of Science and Technology, London, England, 1972.
- [43] Covell, P. F., Wood, R. M., Bauer, S. X., and Walker, I. J., "Configuration Trade and Code Validation Study on a Conical Hypersonic Vehicle," AIAA Paper 85-4505, Sept. 1988.
- [44] Craddock, C., "B-spline Surfaces for CFD Grid Generation," Department of Mechanical Engineering Report 1/95, The University of Queensland, Brisbane, Australia, January 1995.
- [45] Craddock, C. and Jacobs, P., "A Space-Marching Compressible Flow Solver with Chemistry and Optimization," Department of Mechanical Engineering Report 6/98, The University of Queensland, Brisbane, Australia, June 1998.
- [46] Craddock, C. S., Jacobs, P. A., and Gammie, R., "Operational Instructions for the Small Shock Tunnel at UQ," Department of Mechanical Engineering Report 8/98, University of Queensland, July 1998.
- [47] Cresci, R. J., Rubin, S. G., Nardo, C. T., and Lin, T. C., "Hypersonic Interaction along a Rectangular Corner," *AIAA Journal*, Vol. 7, 1969, pp. 2241–2246.
- [48] Curran, E., Heiser, W., and Pratt, D. T., "Fluid Phenomena in Scramjet Combustion Systems," *Annual Review of Fluid Mechanics*, Vol. 28, 1996, pp. 323–360.
- [49] Danberg, J., van Gulick, P., and Kim, J., "Turbulence Modeling for Steady Three-Dimensional Supersonic Flow," Contract Report BRL-CR-553, U.S. Army Ballistic Research Lab., 1986.
- [50] Davies, L. and Wilson, J., "Influence of Reflected Shock and Boundary-Layer Interaction on Shock-Tube Flows," *The Physics of Fluids Supplement*, Vol. 1, 1969, pp. I–37–I–43.

- [51] Davis, R., Barnett, M., and Rakich, J., "The Calculation of Supersonic Viscous Flows Using the Parabolized Navier-Stokes Equations," *Computers and Fluids*, Vol. 14, 1986, pp. 197–224.
- [52] Degani, D. and Schiff, L., "Computation of Turbulent Supersonic Flows around Pointed Bodies Having Crossflow Separation," *Journal of Computational Physics*, Vol. 66, 1986, pp. 173–196.
- [53] DeJong, K., "Genetic Algorithms: a 10 Year Perspective," Proceedings of the First International Conference on Genetic Algorithms., Lawrence Erlbaum, New Jersey, 1985, pp. 169–177.
- [54] Dimotakis, P., "Turbulent Free Shear Layer Mixing and Combustion," In High-Speed Flight Propulsion Systems edited by Murthy, S.N.B and Curran, E.T., AIAA Washington D.C., 1991, pp. 265–340.
- [55] Drummond, J. P., "A Two-Dimensional Numerical Simulation of a Supersonic, Chemically Reacting Mixing Layer," NASA TM-4055, Dec. 1988.
- [56] Ebrahimi, H. B., "CFD Validation For Scramjet Combustor and Nozzle Flows, Part 1," AIAA Paper 93-1840, June 1993.
- [57] Edwards, T. A., "The Effect of Exhaust Plume/Afterbody Interaction on Installed Scramjet Performance," NASA TM 101033, Dec. 1988.
- [58] Edwards, T. A., "Effect of Exhaust Plume/Afterbody Interaction on Installed Scramjet Performance," *Journal of Aircraft*, Vol. 28, No. 2, 1991, pp. 123–130.
- [59] Eleshaky, M. and Baysal, O., "Airfoil Shape Optimization Using Sensitivity Analysis on Viscous Flow Equations," *ASME Journal of Fluids Engineering*, Vol. 117, 1993, pp. 75–84.
- [60] Engblom, W., Yuceil, B., Goldstein, D., and Dolling, D., "Experimental and Numerical Study of Hypersonic Forward-Facing Cavity Flow," *Journal of Spacecraft* and Rockets, Vol. 33, No. 3, 1996, pp. 353–359.
- [61] Evans, J. S. and Schexnayder, C. J. J., "Influence of Chemical Kinetics and Unmixedness on Burning in Supersonic Hydrogen Flames," *AIAA Journal*, Vol. 18, No. 2, 1980, pp. 188–193.
- [62] Evvard, J. C. and Maslen, S. H., "Three-Dimensional Supersonic Nozzles and Inlets of Arbitrary Exit Cross Section," NACA TN 2688, 1952.
- [63] Ferri, A., "Review of Problems in Application of Supersonic Combustion," *Journal of the Royal Aeronautical Society*, Vol. 68, No. 645, 1964, pp. 575–597.

- [64] Ferri, A., "Review of Scramjet Propulsion Technology," *Journal of Aircraft*, Vol. 5, 1968, pp. 3–10.
- [65] Foster, N. and Dulikravich, G., "Three-Dimensional Aerodynamic Shape Optimization Using Genetic and Gradient Search Algorithms," *Journal of Spacecraft and Rockets*, Vol. 34, No. 1, 1997, pp. 36–42.
- [66] Frank, P. and Shubin, G., "A Comparison of Optimization-Based Approaches for a Model Computational Aerodynamic Design Problem," *Journal of Computational Physics*, Vol. 98, 1992, pp. 74–89.
- [67] Freeman, D., Reubush, D., McClinton, C., Rausch, V., and Crawford, J., "The NASA Hyper-X Program," *The 48th International Astronautical Congress*, Turin, Italy, October 1997.
- [68] Garabedian, P. R., Partial Differential Equations, Wiley, New York, 1964.
- [69] Gerbsch, R. and Agarwal, R., "Solution of the Parabolized Navier-Stokes Equations Using Osher's Upwind Scheme," AIAA Paper 90-0392, Jan. 1990.
- [70] Godunov (Ed), S. K., Numerical Solution of Multidimensional Problems in Gasdynamics, Nauka, Moscow, 1976.
- [71] Goldberg, D. E., Genetic Algorithms in Search, Optimization and Machine Learning, Addison-Wesley, Reading, Massachusetts, 1989.
- [72] Goyne, C. P., Stalker, R. J., and Paull, A., "Shock-Tunnel Skin-Friction Measurements in a Supersonic Combustor," *Journal of Propulsion and Power*, Vol. 15, No. 3, 1999.
- [73] Grasso, F. and Magi, V., "Simulation of Transverse Gas Injection in Turbulent Supersonic Air Flows," *AIAA Journal*, Vol. 33, No. 1, 1995, pp. 56–62.
- [74] Gregorenko, V., Naumov, A., and Hvostor, N., "Influence of Non-Stationary Flow Effects on Test Time of a Hypersonic Shock Tunnel," *Scientific Notes of the Central Hydrodynamic Institute*, Vol. 15, No. 5, 1984.
- [75] Griffith, B. J., Maus, J. R., and Majors, B. M., "Addressing the Hypersonic Simulation Problem," *Journal of Spacecraft*, Vol. 24, No. 4, 1987, pp. 334–341.
- [76] Grossman, B. and Cinnella, P., "Flux-split Algorithms for Flows with Nonequilibrium Chemistry and Vibrational Relaxation," *Journal of Computational Physics*, Vol. 88, No. 1, 1990, pp. 131.

- [77] Hackett, C., "Computational and Numerical Analysis of Hypersonic Nozzle Flows with Comparison to Wind Tunnel Calibration Data," AIAA Paper 92-4011, July 1992.
- [78] Haddad, A. and Moss, J. B., "Aerodynamic Design for Supersonic Nozzles of Arbitrary Cross Section," *Journal of Propulsion and Power*, Vol. 6, No. 6, 1990, pp. 740–746.
- [79] Hall, J. and Treanor, C., "Nonequilibrium Effects in Supersonic-Nozzle Flows," AGARDograph 124, 1967, p. 3.
- [80] Hall, J. and Treanor, C., "Nonequilibrium Effects in Supersonic-Nozzle Flows," AGARDograph 124, 1967, pp. 1–95.
- [81] Hall, J. and Treanor, C., "Nonequilibrium Effects in Supersonic-Nozzle Flows," AGARDograph 124, 1967, p. 15.
- [82] Hannemann, K., Jacobs, P. A., Austin, J., Thomas, A., and McIntyre, T., "Transient and Steady-State Flow in a Small Shock Tube," *Proceedings of the 21st International Symposium on Shock Waves, Australia*, AFP Houwing, 1997, p. Paper 2630.
- [83] Harradine, D. M., Lyman, J. L., Oldenborg, R. C., Schott, G. L., and Watanabe,
  H. H., "The Chemical Basis of Efficiency in Hypersonic Flows," *AIAA Journal*,
  Vol. 28, No. 10, 1990, pp. 1740–1744.
- [84] Heiser, W. and Pratt, D., *Hypersonic Airbreathing Propulsion*, AIAA Education Series, Washington, USA, 1994.
- [85] Hilsenrath, J., Tables of Thermodynamic and Transport Properties. National Bureau of Standards. Circular 564; reprinted 1960, Pergamon, New York, 1955.
- [86] Hirsch, C., Numerical Computation of Internal and External Flows. Volume 1: Fundamentals of Numerical Discretization, John Wiley & Sons, 1988.
- [87] Hirsch, C., Numerical Computation of Internal and External Flows. Volume 2: Fundamentals of Numerical Discretization, John Wiley & Sons, 1988, pp. 542.
- [88] Hirschfelder, J., Curtiss, C., and Bird, R., *Molecular Theory of Gases and Liquids*, John Wiley & Sons, New York, 1954.
- [89] Hiscock, S., Kilpin, D., and Drummond, L., "A Versatile Shock Tube and its Analytical Instrumentation," Technical Report 1819(W), Department of Defence, Salisbury, South Australia, 1977.

- [90] Hodge, J. S., Hinson, W. F., and Hackett, C. M., "Description and Calibration of the 31-Inch Mach 10 Wind Tunnel at NASA Langley," Proposed NASA TP, 1994.
- [91] Holden, M. S. and Moselle, J., "Theoretical and Experimental Studies of the Shock Wave-Boundary Layer Interaction on Compression Surfaces In Hypersonic Flow," Report AF-2410-A-1, CALSPAN, Buffalo, New York, 1978.
- [92] Holland, J., *Adaptation in Natural and Artificial Systems*, The University of Michigan Press., 1975.
- [93] Holland, J. H., "Genetic Algorithms," *Scientific American*, Vol. 267, No. 1, 1992, pp. 44–50.
- [94] Homaifar, A., Lai, H., and McCormick, E., "System Optimization of Turbofan Engines using Genetic Algorithms," *Applied Mathematical Modelling*, Vol. 18, 1994, pp. 72–83.
- [95] Horstman, C., "Prediction of Hypersonic Shock-Wave/Turbulent-Boundary- Layer Interaction Flows," AIAA Paper 87-1367, June 1987.
- [96] Huber, P., Schexnayder, C., and McClinton, C., "Criteria for Self-Ignition of Supersonic Hydrogen-Air Mixtures," NASA Technical Paper 1457, 1979.
- [97] Huddleston, D. H., Aerodynamic Design Optimization Using Computational Fluid Dynamics, Ph.D. thesis, University of Tennessee, Knoxville, 1989.
- [98] Hung, C. and MacCormack, R., "Numerical Solution of Three-Dimensional Shock Wave and Turbulent Boundary-Layer Interaction," *AIAA Journal*, Vol. 16, No. 10, 1978, pp. 1090–1096.
- [99] Hung, C. M. and MacCormack, R. W., "Numerical Solutions of Supersonic and Hypersonic Laminar Compression Corner Flows," *AIAA Journal*, Vol. 14, No. 4, 1976, pp. 475–481.
- [100] Ikawa, H., "Rapid Methodology for Design and Performance Prediction of Integrated Supersonic Combustion Ramjet Engines," *Journal of Propulsion and Power*, Vol. 7, No. 3, 1991, pp. 437–444.
- [101] Im, H., Helenbrook, B., Lee, S., and Law, C., "Ignition in the Supersonic Hydrogen/Air Mixing Layer with Reduced Reaction Mechanisms," *Journal of Fluid Mechanics*, Vol. 322, 1996, pp. 275–296.
- [102] Jachimowski, C. J., "An Analytical Study of the Hydrogen-Air Reaction Mechanism With Application to Scramjet Combustion," NASA Technical Paper 2791, 1988.

- [103] Jacobs, P., "L1D: A Computer Program for the Simulation of Transient-flow Facilities," Department of Mechanical Engineering Report 1/99, The University of Queensland, Brisbane, Australia, January 1999.
- [104] Jacobs, P. A., "A Mach 4 Nozzle for Hypervelocity Flow," Department of Mechanical Engineering Report 9/89, University of Queensland, 1989.
- [105] Jacobs, P. A., "Single-Block Navier-Stokes Integrator," NASA Contractor Report 187613, ICASE Interim Report 18, July 1991.
- [106] Jacobs, P. A., "Transient, Hypervelocity Flow in an Axisymmetric Nozzle," AIAA Paper 91-0295, 1991.
- [107] Jacobs, P. A., "An Approximate Riemann Solver for Hypervelocity Flows," AIAA Journal, Vol. 30, No. 10, 1992, pp. 2558–2561.
- [108] Jacobs, P. A., "Quasi-One-Dimensional Modelling of a Free-Piston Shock Tunnel," *AIAA Journal*, Vol. 32, No. 1, 1994, pp. 137–145.
- [109] Jacobs, P. A., "A Space-Marching Euler Solver for Supersonic Flow in a Three-Dimensional Geometry," Department of Mechanical Engineering Report 2/95, The University of Queensland, Brisbane, Australia, January 1995.
- [110] Jacobs, P. A., "MB\_CNS: A Computer Program for the Simulation of Transient Compressible Flows," Department of Mechanical Engineering Report 10/96, The University of Queensland, Brisbane, Dec. 1996.
- [111] Jacobs, P. A. and Craddock, C. S., "Simulation and Optimisation of Heated, Inviscid Flows in Scramjet Ducts," *Journal of Propulsion and Power*, Vol. 15, No. 1, 1999.
- [112] Jacobs, P. A., Macrossan, M. N., and Stalker, R. J., "ARC Collaborative Research Grant, Final Report: Effects of Scale on Scramjet Vehicles," Department of Mechanical Engineering Report 13/96, The University of Queensland, Brisbane, Sept. 1996.
- [113] Jacobs, P. A., Morgan, R. G., Stalker, R. J., and Mee, D. J., "Use of Argon-Helium Driver-Gas Mixtures in the T4 Shock Tunnel," *19th International Symposium on Shock Waves, Marseille, France.*, Springer-Verlag, 1993.
- [114] Jacobs, P. A. and Stalker, R. J., "Design of Axisymmetric Nozzles for Reflected Shock Tunnels," Department of Mechanical Engineering Report 1/89, University of Queensland, 1989.

- [115] Jacobs, P. A. and Stalker, R. J., "Mach 4 and Mach 8 Axisymmetric Nozzles for a High-Enthalpy Shock Tunnel," *The Aeronautical Journal*, Vol. 95, No. 949, 1991, pp. 324–334.
- [116] Jacobs, P. A. and Stalker, R. J., "Mach 4 and Mach 8 Axisymmetric Nozzles for a High-Enthalpy Shock Tunnel," ICASE Report 91-24, 1991.
- [117] Kamath, H., "Parabolized Navier-Stokes Algorithm for Chemically Reacting Flows," AIAA Paper 89-0386, Jan. 1989.
- [118] Keeling, S. L., "A Strategy for the Optimal Design of Nozzle Contours," AIAA Paper 93-2720, July 1993.
- [119] Kerrebrock, J. L., "Some readily Quantifiable Aspects of Scramjet Engine Performance," *Journal of Spacecraft and Rockets*, Vol. 8, No. 5, 1992, pp. 1116–1122.
- [120] Korte, J., "Aerodynamic Design of Axisymmetric Hypersonic Wind-Tunnel Nozzles Using a Least-Squares/Parabolized Navier-Stokes Procedure," *Journal of Spacecraft and Rockets*, Vol. 29, No. 5, 1992, pp. 685–691.
- [121] Korte, J. J., "An Explicit, Upwind Algorithm for Solving the Parabolized Navier-Stokes Equations," Ph. D. Dissertation, North Carolina State University, 1989.
- [122] Korte, J. J., "An Explicit Upwind Algorithm for Solving the Parabolized Navier-Stokes Equations," NASA TP 3050, Feb. 1991.
- [123] Korte, J. J. and Hodge, J. S., "Flow Quality of Hypersonic Wind-Tunnel Nozzles Using Computational Fluid Dynamics," *Journal of Spacecraft and Rockets*, Vol. 32, No. 4, 1995, pp. 569–580.
- [124] Korte, J. J., Kumar, A., Singh, D. J., and Grossman, B., "Least Squares/Parabolized Navier-Stokes Procedure for Optimizing Hypersonic Wind Tunnel Nozzles," AIAA Paper 91-2273, June 1991.
- [125] Korte, J. J., Kumar, A., Singh, D. J., and White, J. A., "CAN-DO, CFD-Based Aerodynamic Nozzle Design and Optimization Program for Supersonic/ Hypersonic Wind Tunnels," AIAA Paper 92-4009, July 1992.
- [126] Korte, J. J. and McRae, D. S., "Explicit Upwind Algorithm for the Parabolized Navier-Stokes Equations," AIAA Paper 88-0716, Jan. 1988.
- [127] Korte, J. J., Singh, D. J., Kumar, A., and Auslender, A. H., "Numerical Study of the Performance of Swept, Curved Compression Surface Scramjet Inlets," *Journal* of Propulsion and Power, Vol. 10, No. 6, 1994, pp. 841–847.
- [128] Krishnamurthy, R., Rogers, R. C., and Tiwari, S. N., "Numerical Study of Hypervelocity Flows Through Scramjet Combustors," *Journal of Propulsion and Power*, Vol. 13, No. 1, 1997, pp. 131–141.
- [129] Kundu, P. K., Fluid Mechanics, Academic Press, New York, 1990, pp. 451.
- [130] Kuruvila, G., Ta'asan, S., and Salas, M., "Airfoil Design and Optimization by the One-Shot Method," AIAA Paper 95-0478, Jan. 1995.
- [131] Lawrence, S. L., Chaussee, D. S., and Tannehill, J. C., "Development of a Three-Dimensional Upwind Parabolized Navier-Stokes Code," *AIAA Journal*, Vol. 28, No. 6, 1990, pp. 971–972.
- [132] Lawrence, S. L., Tannehill, J. C., and Chaussee, D. S., "Upwind Algorithm for the Parabolized Navier-Stokes Equations," *AIAA Journal*, Vol. 27, No. 9, 1989, pp. 1175–1183.
- [133] Lee, J., "Basic Governing Equations for the Flight Regimes of Aeroassisted Orbital Transfer Vehicles. *Thermal Design of Aeroassisted Orbital Transfer Vehicles*," *Volume 96 of Progress in Astronautics and Aeronautics*, edited by H. Nelson, AIAA, 1985, pp. 3–53.
- [134] Liepmann, H. W. and Roshko, A., *Elements of Gasdynamics*, John Wiley and Sons, New York, 1957.
- [135] Lin, R. S., Edwards, J. R., Wang, W. P., and Malik, M. R., "Instabilities of a Mach 2.4 Slow-Expansion Square Nozzle Flow," AIAA Paper 96-0784, Jan. 1996.
- [136] Lin, T. and Rubin, S., "A Numerical Model for Supersonic Viscous Flow Over a Slender Reentry Vehicle," AIAA Paper 79-0205, 1979.
- [137] Liou, M. S. and Steffen, C. J., "A New Flux Splitting Scheme," NASA TM 104404, 1991.
- [138] Lockwood O'Neill, M. K. and Lewis, M. J., "Design Tradeoffs on Scramjet Engine Integrated Hypersonic Waverider Vehicles," *Journal of Aircraft*, Vol. 30, No. 6, 1993, pp. 943.
- [139] Lubard, S. C. and Helliwell, W. S., "Calculation of the Flow on a Cone at High Angle of Attack," *AIAA Journal*, Vol. 12, No. 7, 1974, pp. 965–974.
- [140] Mace, J. and Hankey, W., "Review of Inlet-Airframe Integration Using Navier-Stokes Computational Fluid Dynamics," AIAA Paper 84-0119, 1984.

- [141] Mager, A., "On the Model of the Free, Shock-Separated Turbulent Boundary Layer," *Journal of the Aeronautical Sciences*, Vol. 23, No. 2, 1956, pp. 181–184.
- [142] Mahoney, J., Inlets for Supersonic Missiles, AIAA, Washington, 1990, pp. 80.
- [143] Mahoney, J., Inlets for Supersonic Missiles, AIAA, Washington, 1990, pp. 47.
- [144] Mahoney, J., Inlets for Supersonic Missiles, AIAA, Washington, 1990, pp. 73.
- [145] Martin, R. S. and Wilkinson, J. H., "Solution of Symmetric and Unsymmetric Band Equations and the Calculation of Eigenvectors of Band Matrices," *Numerische Mathematik*, 1967, pp. 279–301.
- [146] Matsuzaki, R. and Hirabayashi, N., "Predictions of Temperatures and Velocity in a Nonequilibrium Nozzle Flow of Air," AIAA Paper 87-1477, June 1987.
- [147] McBride, B., Gordon, S., and Reno, M., "Thermodynamic Data for Fifty Reference Elements," NASA Technical Paper 3287, 1993.
- [148] McQuade, P. D., Eberhardt, S., and Livne, E., "CFD-Based Aerodynamic Approximation Concepts Optimization of a Two-Dimensional Scramjet Vehicle," *Journal* of Aircraft, Vol. 32, No. 2, 1995, pp. 262–269.
- [149] Michalewicz, Z. and Janikow, C. Z., "Genetic Algorithms for Numerical Optimization," *Statistics and Computing*, Vol. 1, 1991, pp. 75–91.
- [150] Micol, J. R., "Hypersonic Aerodynamic/Aerothermodynamic Testing Capabilities at Langley Research Center: Aerothermodynamic Facilities Complex," AIAA Paper 95-2107, June 1995.
- [151] Miller, C. G., "Measured Pressure Distributions, Aerodynamic Coefficients, and Shock Shapes on Blunt Bodies at Incidence in Hypersonic Air and CF<sub>4</sub>," NASA TM-84489, Sept. 1982.
- [152] Miller, C. G., "Langley Hypersonic Aerodynamic/Aerothermodynamic Testing Capabilities – Present and Future," AIAA Paper 90-1376, June 1990.
- [153] Miller, C. G. and Smith, F. M., "Langley Hypersonic Facilities Complex Description and Application," AIAA Paper 86-0741-CP, March 1986.
- [154] Millikan, R. and White, D., "Systematics of Vibrational Relaxation," *Journal of Chemical Physics*, Vol. 39, No. 12, 1963, pp. 3209–3213.
- [155] Morel, T., "Design of Two-Dimensional Wind Tunnel Contractions." AMSE Journal of Fluids Engineering, 1977, pp. 371–378.

- [156] Morrison, J. H. and Korte, J. J., "Implementation of Vigneron's Streamwise Pressure Gradient Approximation in Parabolized Navier-Stokes Equations," *AIAA Journal*, Vol. 30, No. 11, 1992, pp. 2774–2776.
- [157] Murman, E. M., "Analysis of Embedded Shock Waves Calculated by Relaxation Methods," *AIAA Journal*, Vol. 12, No. 5, 1974, pp. 626–633.
- [158] National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, and United States Air Force, U.S. Standard Atmosphere, NASA, 1962.
- [159] Nelder, J. A. and Mead, R., "A Simplex Method for Function Minimization," *Computer Journal*, Vol. 7, 1965, pp. 338–345.
- [160] Neufeld, P., Janzen, A., and Aziz, R., "Empirical Equations to Calculate 16 of the Transport Collision Integrals for the Lennard-Jones (12-6) Potential," *The Journal* of Chemical Physics, Vol. 57, No. 3, 1972, pp. 1100–1102.
- [161] Northam, G. B. and Anderson, G. Y., "Supersonic Combustion Ramjet Research at Langley," AIAA Paper 86-0159, 1986.
- [162] Obayashi, S. and Tsukahara, T., "Comparison of Optimization Algorithms for Aerodynamic Shape Design," *AIAA Journal*, Vol. 35, No. 8, 1993, pp. 1413–1415.
- [163] Oldenborg, R. and *et al.*, "Hypersonic Combustion Kinetics : Status Report of the Rate Constant Committee, NASP High-Speed Propulsion Technology Team," NASP Technical Memorandum 1107, May 1990.
- [164] Olsson, D. M. and Nelson, L. S., "The Nelder-Mead Simplex Procedure for Function Minimization," *Technometrics*, Vol. 17, No. 1, 1975, pp. 45–51.
- [165] O'Neill, R., "Algorithm AS47. Function Minimization Using a Simplex Algorithm," *Applied Statistics*, Vol. 20, 1971, pp. 338–345.
- [166] Osher, S. and Chakravarthy, S., "Upwind Schemes and Boundary Conditions with Applications to Euler Equations in General Geometries," *Journal of Computational Physics*, Vol. 50, 1983, pp. 447–481.
- [167] Osher, S. and Solomon, F., "Upwind Difference Schemes for Hyperbolic Systems of Conservation Laws," *Mathematics of Computation*, Vol. 38, No. 158, 1982, pp. 339–374.
- [168] Ostrander, M. J., Thomas, S. R., Voland, R. T., Guy, R. W., and Srinivasan, S., "CFD Simulations of Square Cross-Section, Contoured Nozzle Flows: Comparison With Data," AIAA Paper 89-0045, Jan. 1989.

- [169] Park, C., "Assessment of Two-Temperature Kinetic Model for Ionizing Air," AIAA Paper 87-1574, June 1987.
- [170] Parker, L. J., Cave, M., and Barnes, R., "Comparison of Simplex Algorithms," *Analytica Chimica Acta*, Vol. 175, 1985, pp. 231–237.
- [171] Prabhu, R. and Erickson, W., "A Rapid Method for the Computation of Equilibrium Chemical Composition of Air to 15000K," NASA Technical Paper 2792, 1988.
- [172] Pruett, C. D. and Streett, C. L., "A Spectral Collocation Method for Compressible, Non-Similar Boundary Layers," *International Journal for Numerical Methods in Fluids*, Vol. 13, No. 6, 1991, pp. 713–737.
- [173] Rao, G., "Exhaust Nozzle Contour for Maximum Thrust," *Jet Propulsion*, Vol. 28, No. June, 1958, pp. 377–382.
- [174] Reid, R., Prausnitz, J., and Poling, B., *The Properties of Gases and Liquids: 4th edition.*, McGraw Hill, New York, 1987.
- [175] Riggins, D. W., "Thrust Losses in Hypersonic Engines Part 2: Applications," *Journal of Propulsion and Power*, Vol. 13, No. 2, 1997, pp. 288–295.
- [176] Riggins, D. W., McClinton, C. R., Rogers, R. C., and Blittner, R. D., "Investigation of Scramjet Injection Strategies for High Mach Number Flows," *Journal of Propulsion and Power*, Vol. 11, No. 3, 1995, pp. 409–418.
- [177] Riggins, D. W., McClinton, C. R., and Vitt, P. H., "Thrust Losses in Hypersonic Engines Part 1: Methodology," *Journal of Propulsion and Power*, Vol. 13, No. 2, 1997, pp. 281–295.
- [178] Riggins, D. W. and Vitt, P. H., "Vortex Generation and Mixing in Three-Dimensional Supersonic Combustors," *Journal of Propulsion and Power*, Vol. 11, No. 3, 1995, pp. 419–426.
- [179] Rizzi, A. W. and Inouye, M., "Time-Split Finite-Volume Method for Three-Dimensional Blunt-Body Flow," AIAA Journal, Vol. 11, No. 11, 1973, pp. 1478– 1485.
- [180] Roache, P. J., "A Method for Uniform Reporting of Grid Refinement Studies," *Journal of Fluids Engineering*, Vol. 116, 1994, pp. 405–413.
- [181] Roe, P. L., "Approximate Riemann Solvers, Parameter Vectors, and Difference Schemes," *Journal of Computational Physics*, Vol. 43, 1981, pp. 357–372.

- [182] Rogers, D. F. and Adams, J. A., *Mathematical Elements for Computer Graphics* (2nd ed.), McGraw-Hill, New York, 1990.
- [183] Rogers, R. C. and Chinitz, W., "Using a Global Hydrogen-Air Combustion Model in Turbulent Reacting Flow Calculations," *AIAA Journal*, Vol. 21, 1983, pp. 586– 592.
- [184] Roudakov, A. S., Semenov, V. L., and Hicks, J. W., "Recent Flight Test Results of the Joint CIAM-NASA Mach 6.5 Scramjet Flight Program," AIAA Paper 98-1643, April 1998.
- [185] Routh, M., Schwartz, P., and Denton, M., "Performance of the Super Modified Simplex," *Analytical Chemistry*, Vol. 49, 1977, pp. 1422.
- [186] Rubin, T. D. and Lin, T., "A Numerical Method for Three-Dimensional Viscous Flow: Application to the Hypersonic Leading Edge Equations," *Journal of Computational Physics*, Vol. 9, 1972, pp. 339–364.
- [187] Rubin, T. D. and Lin, T., "Marching with the PNS Equations," *Proceeding of 22nd Israel Annual Conference on Aviation and Astronautics*, 1980, pp. 60–61.
- [188] Rudman, S. and Rubin, F., "Hypersonic Viscous Flow over Slender Bodies with Sharp Leading Edges," *AIAA Journal*, Vol. 6, 1968, pp. 1883–1890.
- [189] Rudy, D. H., Kumar, A., Gnoffo, P. A., and Chakravarthy, S. R., "A Validation Study of Four Navier-Stokes Codes for High-Speed Flows," AIAA Paper 89-1838, 1989.
- [190] Rudy, D. H., Thomas, J. L., Kumar, A., Gnoffo, P. A., and Chakravarthy, S. R., "Computation of Laminar Hypersonic Compression-Corner Flows," *Annual Review of Fluid Mechanics*, Vol. 29, No. 7, 1991, pp. 1108–1113.
- [191] Sabean, J. w. and Lewis, M. J., "Performance Optimization of a Supersonic Combustion Ram Accelerator Projectile," *Journal of Propulsion and Power*, Vol. 13, No. 5, 1997, pp. 592–600.
- [192] Salomon, R., "Raising Theoretical Questions About the Utility of Genetic Algorithms," *Evolutionary Programming VI, Lecture Notes in Computer Science, 1213*, Springer-Verlag, 1997, pp. 275–284.
- [193] Scales, L., Introduction to Non-Linear Optimization., Macmillan, London, 1985.
- [194] Schiff, L. B. and Steger, W. B., "Numerical Simulation of Steady Supersonic Viscous Flow," AIAA Paper 79-0130, Jan. 1979.

- [195] Shirazi, S. and Truman, C., "Evaluation of Algebraic Turbulence Models for PNS Predictions of Supersonic Flow Past a Sphere-Cone," *AIAA Journal*, Vol. 27, No. 5, 1989, pp. 560–568.
- [196] Siclari, M. J. and Del Guidice, P., "Hybrid Finite Volume Approach to Euler Solutions for Supersonic Flows," *AIAA Journal*, Vol. 28, No. 1, 1990, pp. 66–74.
- [197] Sivells, J. C., "Aerodynamic Design of Axisymmetric Hypersonic Wind Tunnel Nozzles," *Journal of Spacecraft and Rockets*, Vol. 7, No. 11, 1970, pp. 1292–1299.
- [198] Slack, M. and Grillo, A., "Investigation of Hydrogen Air Ignition Sensitized by Nitric Oxide and by Nitrogen Dioxide," NASA CR-2896, 1993.
- [199] Smith, C. E., "The Starting Process in a Hypersonic Nozzle," Journal of Fluid Mechanics, Vol. 24, 1966, pp. 625–640.
- [200] Spendley, W., Hext, G., and Himsworth, F., "Sequential Application of Simplex Designs in Optimisation and Evolutionary Operation," *Technometrics*, Vol. 4, 1962, pp. 441.
- [201] Srinivas, K., "An Explicit Spatial Marching Algorithm for Navier-Stokes Equations," *Computers and Fluids*, Vol. 21, No. 2, 1992, pp. 291–299.
- [202] Srinivas, K., "An Explicit Finite Volume Spatial Marching Method for Reduced Navier-Stokes Equations," *International Journal for Numerical Methods in Fluids*, Vol. 22, 1995, pp. 121–135.
- [203] Srinivasan, S., Tannehill, J. C., and Weilmuenster, K. J., "Simplified Curve Fits for the Thermodynamic Properties of Equilibrium Air," NASA Reference Publication 1181, 1987.
- [204] Stalker, R., "A Study of the Free-Piston Shock Tunnel," AIAA Journal, Vol. 5, No. 12, 1967, pp. 2160–2165.
- [205] Stalker, R., "Hypervelocity Aerodynamics with Chemical Nonequilibrium," Annual Review of Fluid Mechanics, Vol. 21, 1989, pp. 37–60.
- [206] Stalker, R. and Crane, K., "Driver Gas Contamination in a High Enthalpy Reflected Shock Tunnel," *AIAA Journal*, Vol. 16, No. 3, 1978, pp. 277–279.
- [207] Stalker, R. and Morgan, R., "The University of Queensland Free Piston Shock Tunnel T4 - Initial Operation and Preliminary Calibration," *Fourth National Space Engineering Symposium, Adelaide, Australia*, IEAust, 1988.

- [208] Stalker, R. J., "Waves and Thermodynamics in High Mach Number Propulsive Ducts," *In High-Speed Flight Propulsion Systems edited by Murthy, S.N.B and Curran, E.T.*, AIAA Washington D.C., 1991, pp. 237–264.
- [209] Stalker, R. J., "Scaling Laws and the Launch Vehicle Market," *Seventh National Space Engineering Symposium, Canberra*, 1992.
- [210] Steger, J. L. and Warming, R. F., "Flux Vector Splitting of the Inviscid Gasdynamic Equations with Applications to Finite-Difference Methods," *Journal of Computational Physics*, Vol. 40, 1981, pp. 263–293.
- [211] Sutherland, W., "The Viscosity of Gases and Molecular Force," *Phil. Mag.*, Vol. 5, 1983, pp. 507–531.
- [212] Svehla, R. A., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA Technical Paper R-132, Lewis Research Center, Washington, DC, 1962.
- [213] Swanson, R. C., Turkel, E., and White, J. A., "An Effective Multigrid Method for High-Speed Flows," *Fifth Copper Mountain Conference on Multigrid Methods*, 1991.
- [214] Sweby, P. K., "High Resolution Schemes using Flux Limiters for Hyperbolic Conservation Laws," SIAM J. Numer. Anal., Vol. 21, 1984, pp. 995–1010.
- [215] Swithenbank, J., "Hypersonic Air-Breathing Propulsion," Progresses in Aeronautical Sciences, Vol. 8, 1966, pp. 229–294.
- [216] Tannehill, J., Venkatapathy, E., and Rakich, J., "Numerical Solution of Supersonic Viscous Flow over Blunt Delta Wings," *AIAA Journal*, Vol. 20, No. 2, 1982, pp. 203–210.
- [217] Tannehill, J. C., Anderson, D. A., and Pletcher, R. H., Computational Fluid Mechanics and Heat Transfer: Second Edition, Taylor & Francis Publishers, Washington, DC, 1997, pp. 563.
- [218] Tannehill, J. C., Anderson, D. A., and Pletcher, R. H., Computational Fluid Mechanics and Heat Transfer: Second Edition, Taylor & Francis Publishers, Washington, DC, 1997, pp. 375–398.
- [219] Tannehill, J. C., Anderson, D. A., and Pletcher, R. H., Computational Fluid Mechanics and Heat Transfer: Second Edition, Taylor & Francis Publishers, Washington, DC, 1997, pp. 253.

- [220] Tannehill, J. C., Anderson, D. A., and Pletcher, R. H., Computational Fluid Mechanics and Heat Transfer: Second Edition, Taylor & Francis Publishers, Washington, DC, 1997, pp. 337.
- [221] Thomas, S. R., Voland, R. T., and Guy, R. W., "Test Flow Calibration Study of the Langley Arc-Heated Scramjet Test Facility," AIAA Paper 87-2165, June 1987.
- [222] Tolle, R., "A New Optimum Design Code for Hypersonic Nozzles, Utilizing Response Surface Methodology," AIAA Paper 97-0519, Jan. 1997.
- [223] Toro, E. F., "A Fast Riemann Solver with Constant Covolume Applied to the Random Choice Method," *International J. for Numerical Methods in Fluids*, Vol. 9, 1989, pp. 1145–1164.
- [224] Toro, E. F., "A Linearized Riemann Solver for the Time-Dependent Euler Equations of Gas Dynamics," Proc. Roy. Soc. London, Vol. A 434, 1991, pp. 683–693.
- [225] Tracy, R. R., "Hypersonic Flow Over a Yawed Circular Cone," Aeronautical Laboratories Memorandum 69, California Institute of Technology, 1963.
- [226] van Leer, B., "Towards the Ultimate Conservative Difference Scheme. V. A Second-Order Sequel to Godunov's Method," *Journal of Computational Physics*, Vol. 32, 1979, pp. 101–136.
- [227] van Leer, B., "Flux-Vector Splitting for the Euler Equations," *Lectures Notes in Physics, Volume 170.*, Springer-Verlag, 1982, pp. 507–512.
- [228] Vigneron, Y. C., Rakich, J. V., and Tannehill, J. C., "Calculation of Supersonic Viscous Flow over Delta Wings with Sharp Subsonic Leading Edges," AIAA Paper 78-1137, July 1978.
- [229] Vinokur, M., "An Analysis of Finite-Difference and Finite-Volume Formulations of Conservation Laws," NASA CR 177416, 1986.
- [230] Voland, R. T., Rock, K., Huedner, L., Witte, D., Fischer, K., and McClinton, C., "Hyper-X Engine Design and Ground Test Program," AIAA Paper 98-1532, April 1998.
- [231] Vuong, S. and Coakley, T., "Modeling of Turbulence for Hypersonic Flows With and Without Separation," AIAA Paper 87-0286, Jan. 1987.
- [232] Wadawadigi, G., Tannehill, J. C., Buelow, P. E., and Lawrence, S. L., "Three-Dimensional Upwind Parabolized Navier-Stokes Code for Supersonic Combustion Flowfields," *Journal of Thermophysics and Heat Transfer*, Vol. 7, No. 4, 1993, pp. 661–667.

- [233] Weber, R. J. and MacKay, J., "An Analysis of Ramjet Engines Using Supersonic Combustion," NACA TN 4386, 1958.
- [234] Wendt, M. N. and Jacobs, P. A., "Modular Composite Scramjet Motor (C.S.M) Testing," Department of Mechanical Engineering Report 2/96, The University of Queensland, Brisbane, Australia, February 1996.
- [235] West, J. E. and Korkegi, R. H., "Supersonic Interaction in the Corner of Intersecting Wedges at High Reynolds Numbers," *AIAA Journal*, Vol. 10, No. 5, 1972, pp. 652– 656.
- [236] White, F. M., Viscous Fluid Flow., McGraw-Hill, New York, 1974, Figure 7-4.
- [237] White, S. C., "Characterising a Mach Seven Nozzle for a Shock Tunnel," Undergraduate Thesis, University of Queensland, 1997.
- [238] Wilke, C. R., "A Viscosity Equation for Gas Mixtures," *Journal of Chemical Physics*, Vol. 18, 1950, pp. 517–519.
- [239] Yokota, K. and Kaji, S., "Two and Three Dimension Study on Supersonic Flow and Mixing Fields with Hydrogen Injection," AIAA Paper 95-6024, April 1995.
- [240] Zanchetta, M. and Cain, T., "An Axisymmetric Internal Compression Inlet," AIAA Paper 98-1525, April 1998.
- [241] Zonars, D., "Nonequilibrium Regime of Airflows in Contoured Nozzles : Theory and Experiment," *AIAA Journal*, Vol. 5, No. 1, 1967, pp. 57–63.