Numerical Investigation of Shock Stand-off in Chlorine

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Ballistic range experiments

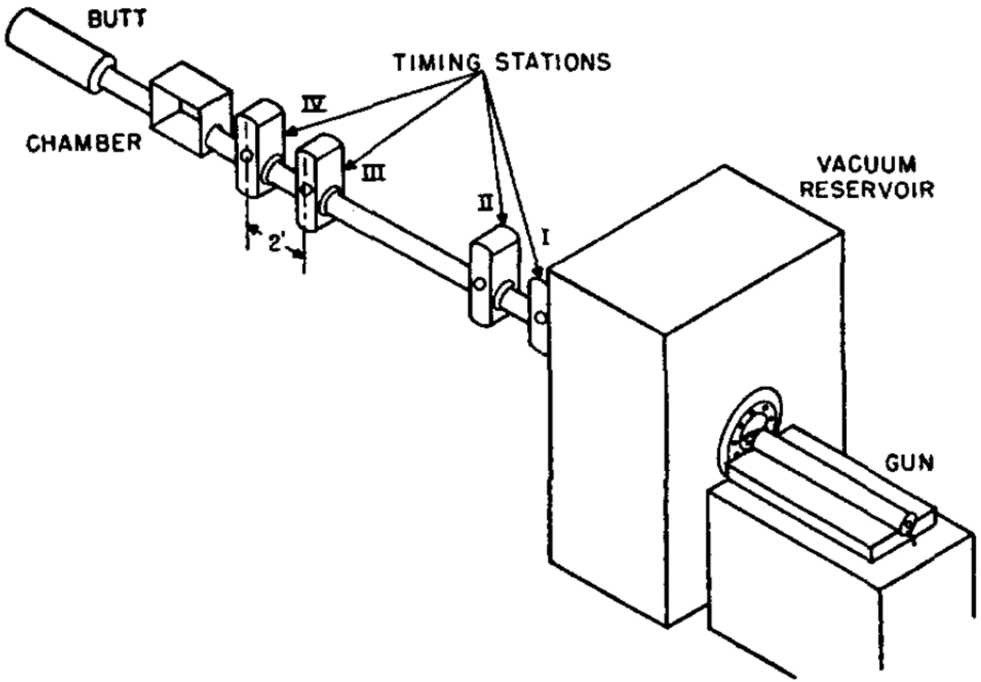
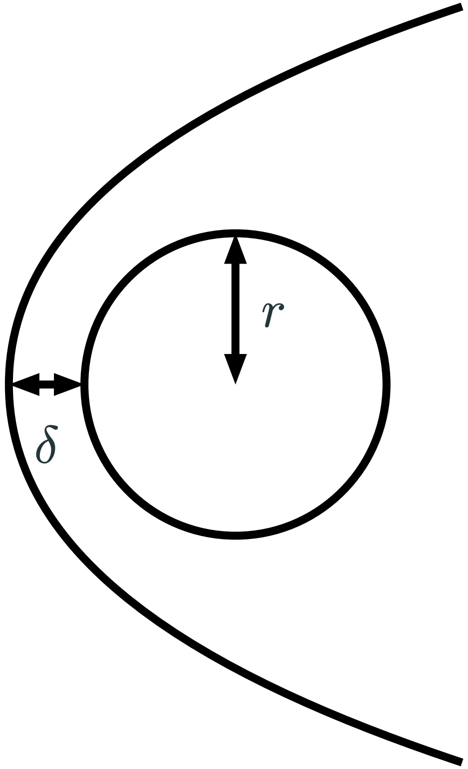


Figure 1: Schematic of ballistic range from Schwartz and Eckerman[1]

- Performed by Schwartz and Eckerman in 1956[1]
- Aim of experiment:
  - Measure vibrational relaxation of Cl_2 by measuring shock stand-off distance
- Gun tunnel
  - 4 mm radius ball bearings, various materials
  - Schlieren/shadowgraphs to measure shock stand-off distance
- Hopefully good for CFD validation
  - Isolates vibrational relaxation (e.g. no dissociation, electronic excitation e.g.)

[1] Schwartz and Eckerman, 1956: *Shock Location in Front of a Sphere as a Measure of Real Gas Effects*

Measurements



- Measurements of shock stand-off distance at various Mach numbers (2-4) and pressures ($\sim$ 130 Pa through $\sim$ 25 kPa)
- The level of vibrational nonequilibrium changes γ, which changes shock stand-off
- Matching shock stand-off in CFD requires getting vibrational relaxation correct

Gas Dynamics Toolkit[1]

GDTk is a collection of software for doing gas dynamics, from simple desktop calculations through to simulations on supercomputers

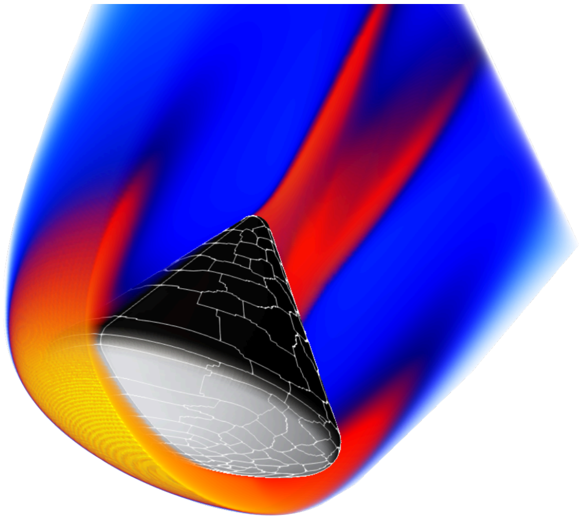
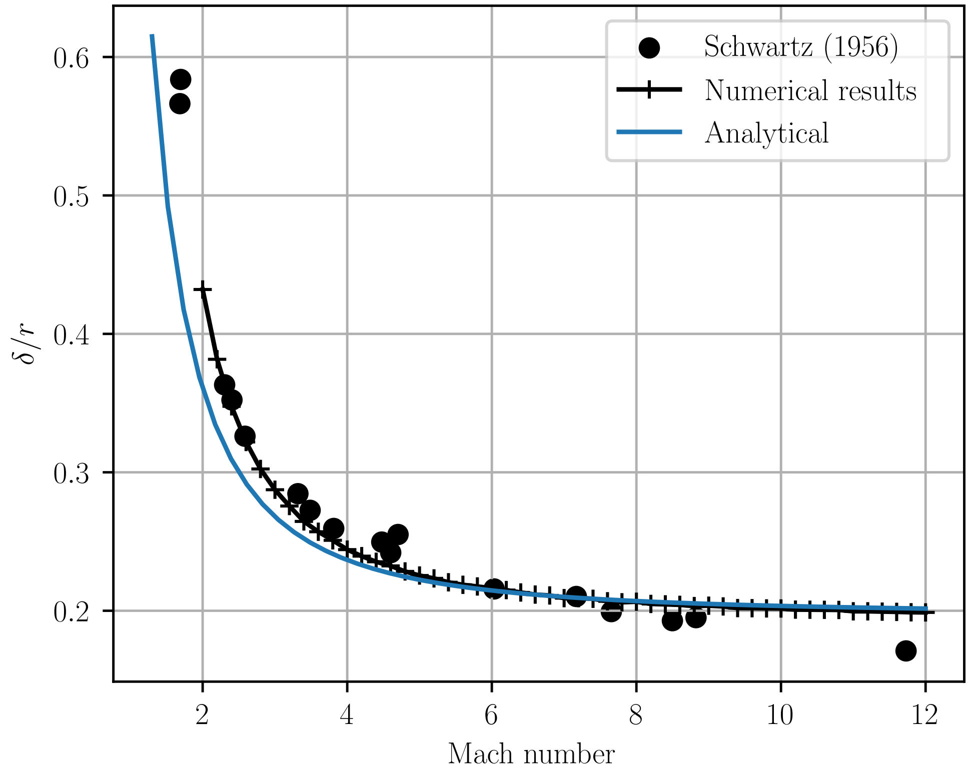
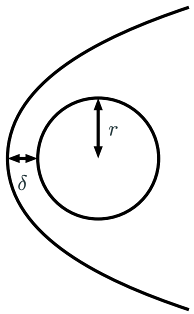


Figure 2: Simulation of Apollo capsule with Eilmer

https://gdtk.uqcloud.net

[1] Gibbons *et. al.*, 2023: *Eilmer: An open-source multi-physics hypersonic flow solver*

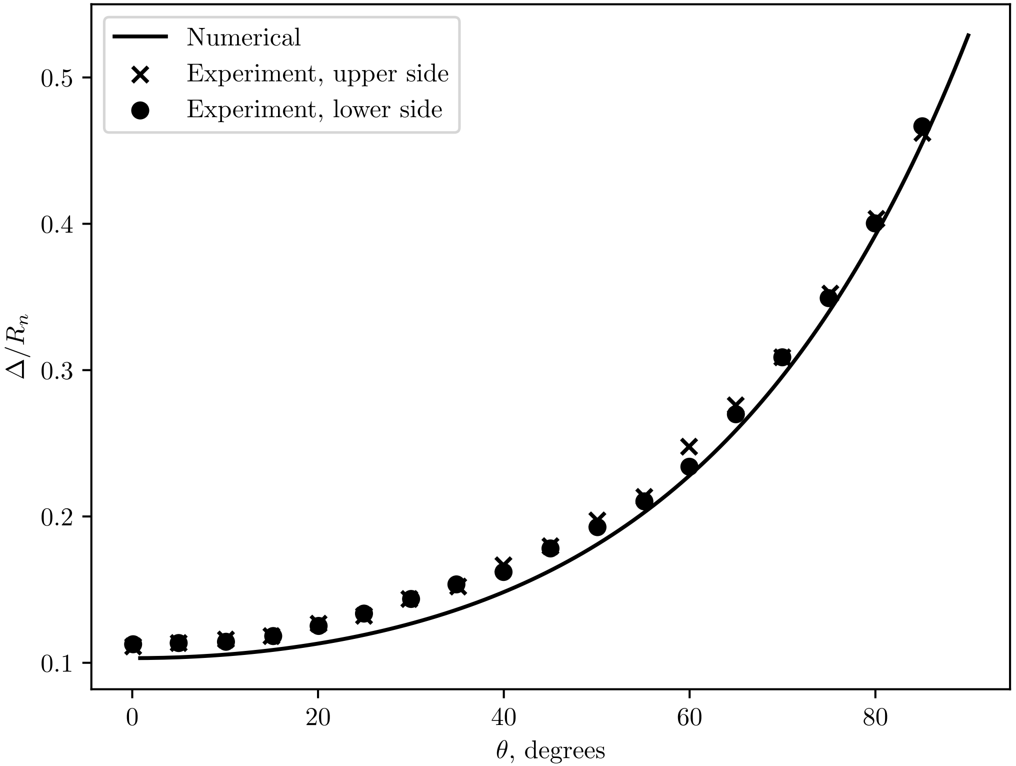


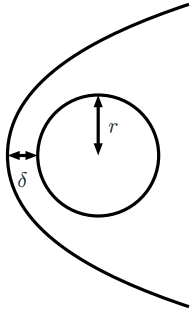


- Validation of the experimental setup
- Validation of the `Eilmer`[1]

[1] Gollan and Jacobs, 2013: *About the formulation, verification and validation of the hypersonic flow solver Eilmer*

Nonaka Sphere - Separate validation of Eilmer





- Shock shape validation with the Nonaka Sphere[1] in air
- Full thermochemical nonequilibrium is required to get the correct shock shape

[1]Nonaka *et. al.*, 2012: *Measurement of shock stand-off distance for sphere in ballistic range*

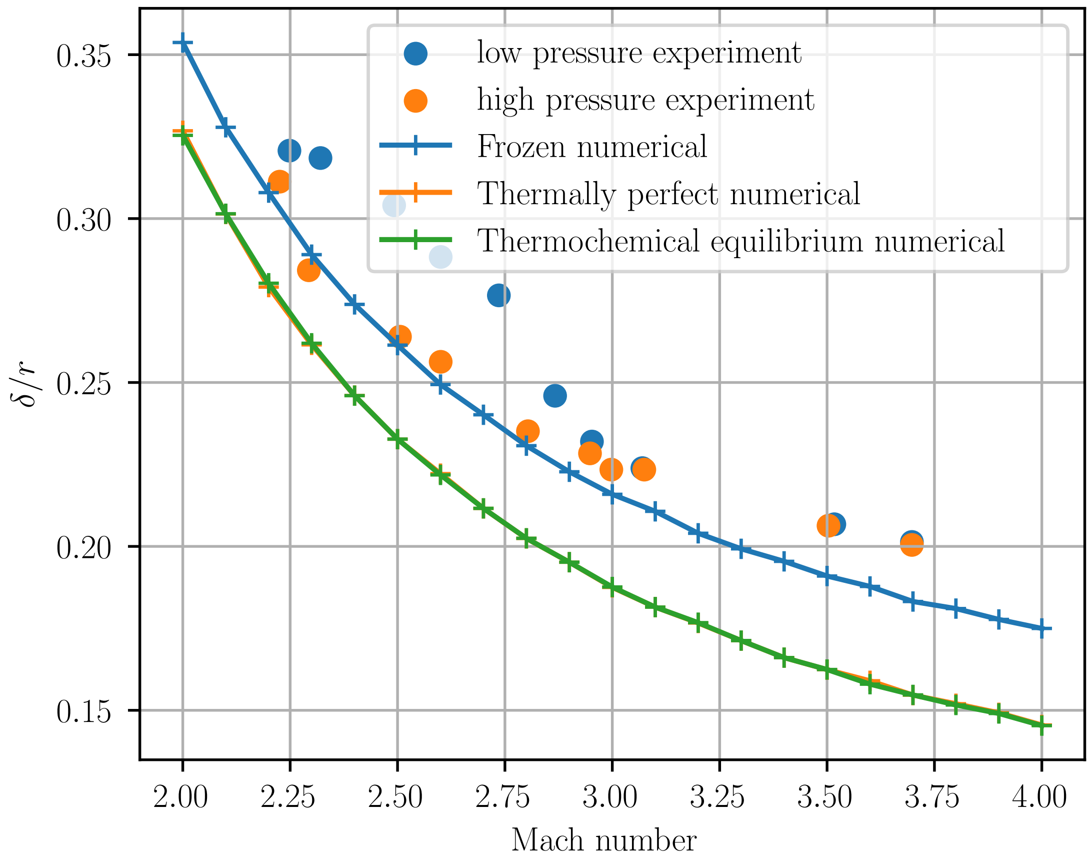
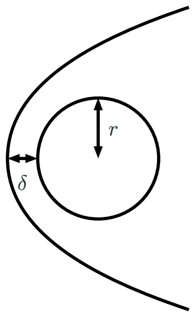
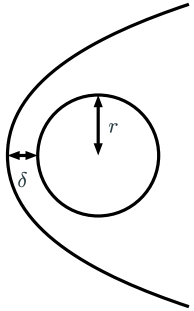


Figure 5: Chlorine shock stand-off distance



- Results from over a decade ago
- Frozen and equilibrium assumptions do not bound experimental results



Numerics

- Second-order finite-volume
- body-fitted grid
- Jacobian-Free Newton-Krylov for steady-state acceleration

Gas Models

- Ideal Cl_2
- Thermally perfect Cl_2
- Equilibrium mixture of Cl_2 and Cl
  - Equilibrium computed with Nick Gibbons' `eqc`

Simulations

- Half sphere, 2D axisymmetric
- Initial inviscid shock-fit solution
- Four successive viscous solutions on finer grids
  - Finest grid: 210×210 with first cell $1\mu m$
  - Grid is tailored to align with the shock of each simulation
- 20 Simulations from Mach 2-4, for each gas model

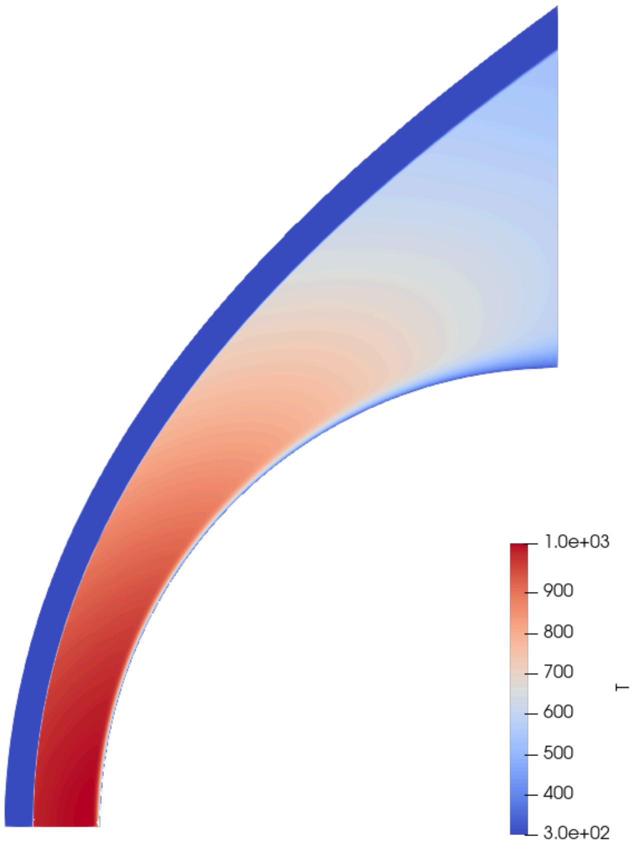
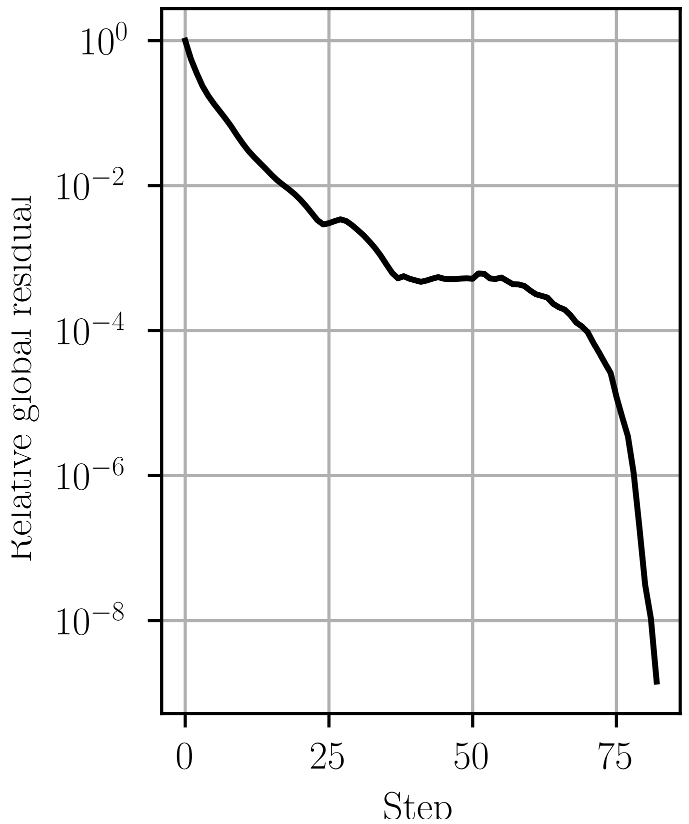


Figure 6: Representative flow field



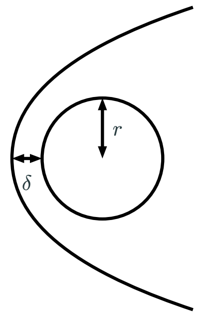
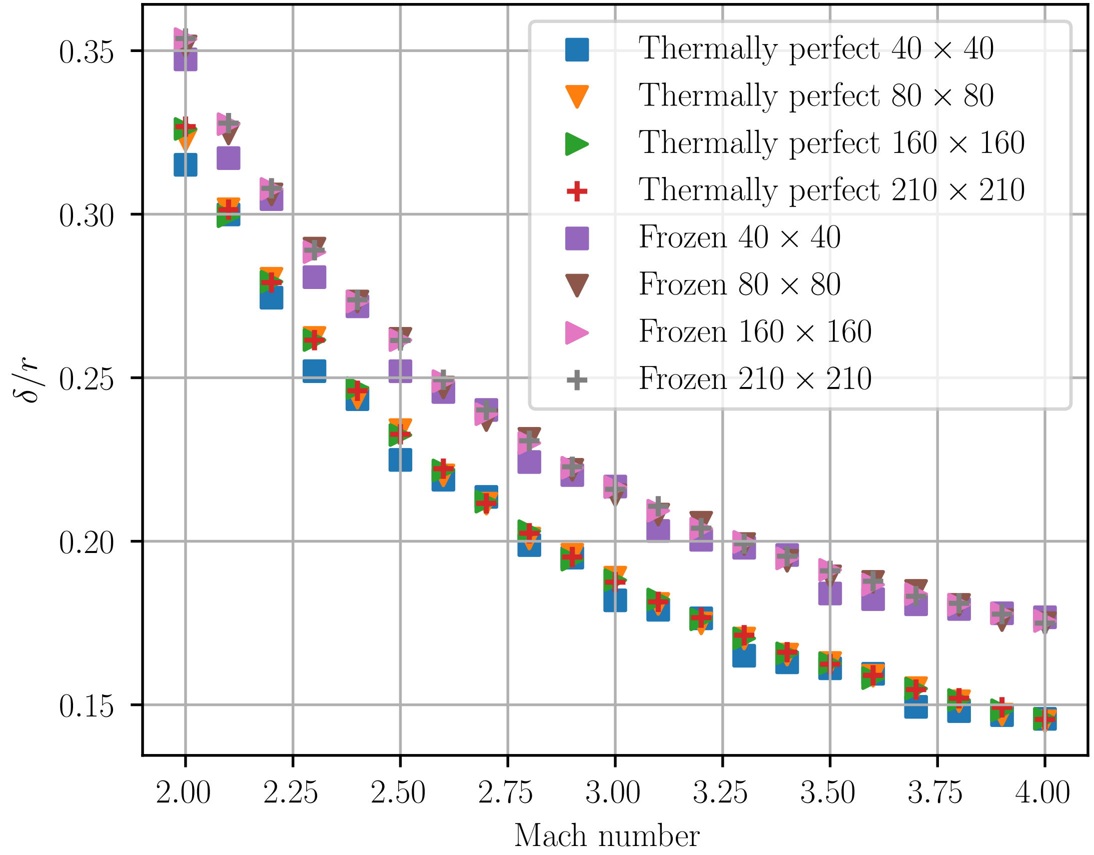
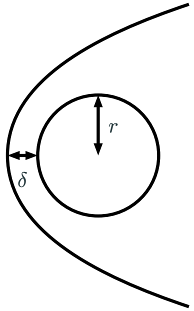


Figure 7: Representative convergence

Grid Convergence





Chlorine results

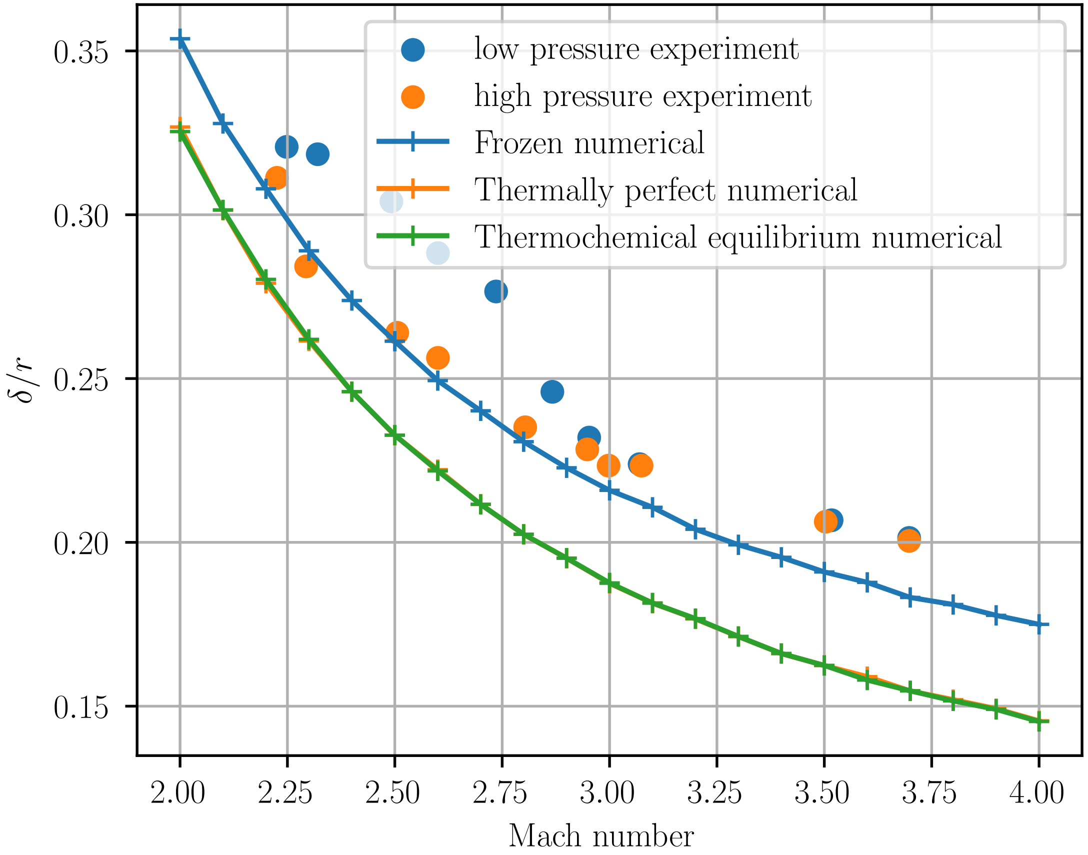
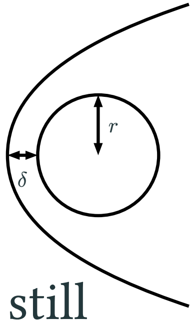


Figure 9: Comparison of simulated and observed shock stand-off



- Numerical shock stand-off is still too small
- Require *effective* γ to increase
  - Rules out Cl_2 reacting and forming more complex molecules
  - Rules out contamination with oil or grease from the gun
- Or require speed to decrease

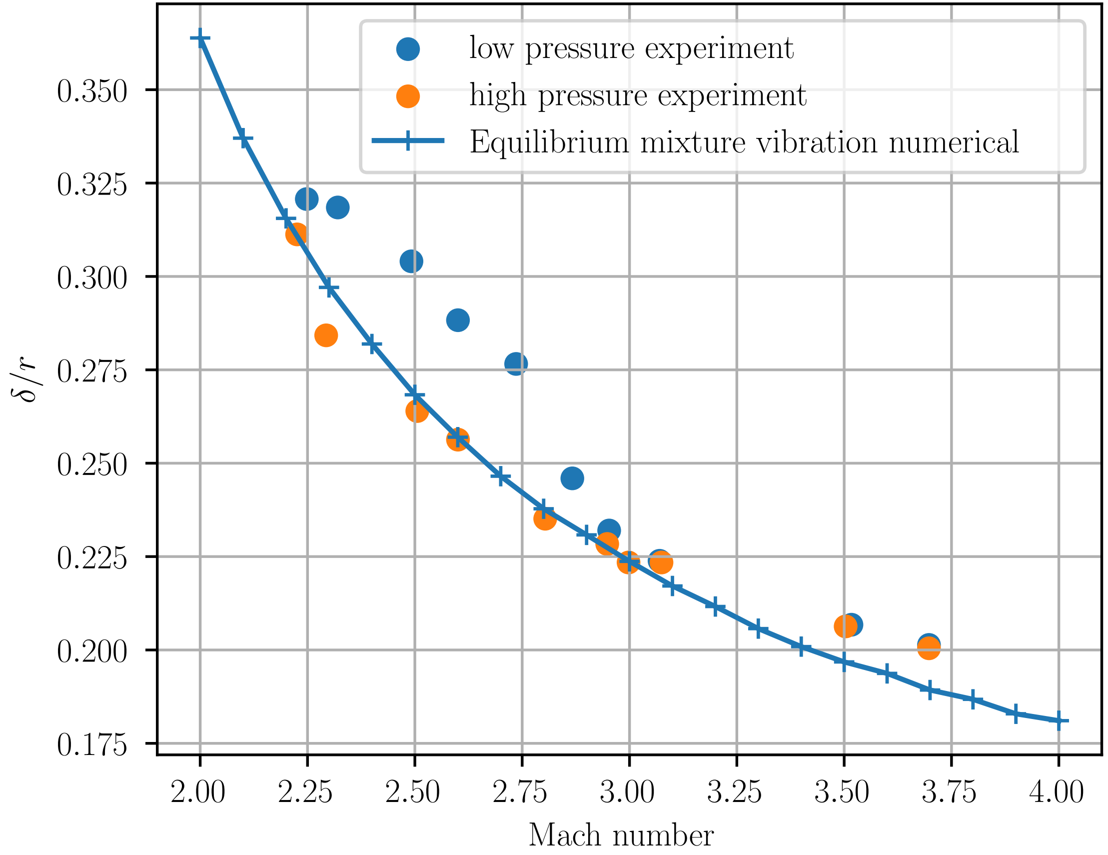
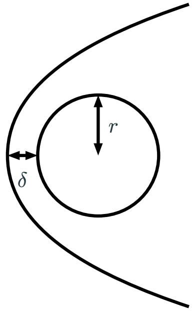
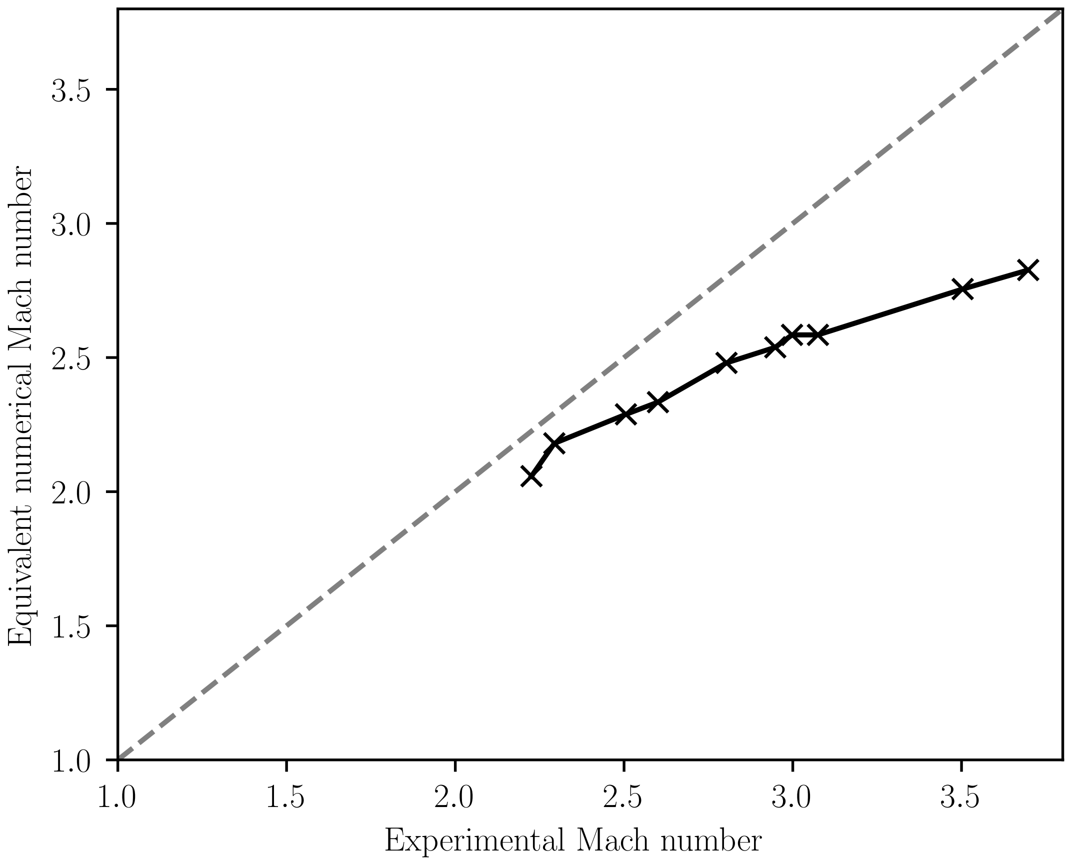


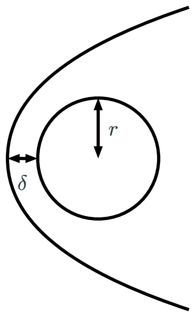
Figure 10: Mixture of Ar and Cl_2



- Thermally perfect gas model
- 60% Cl_2, 40% Ar by mass
  - $\gamma_{\text{effective}} \approx 1.42$
- Unrealistic for there to be so much contamination

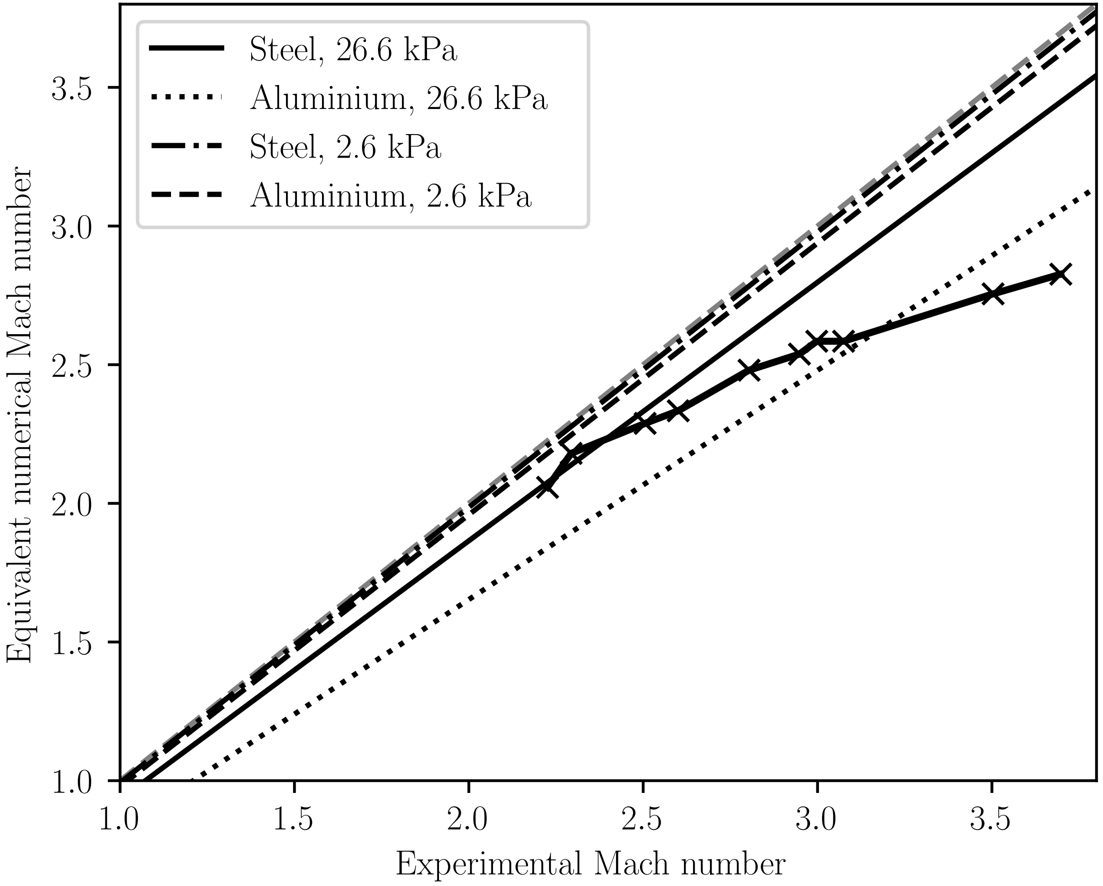
Deceleration

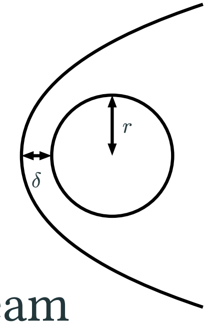




- Calculate the free-stream speed to get the same numerical shock stand-off as the experiment

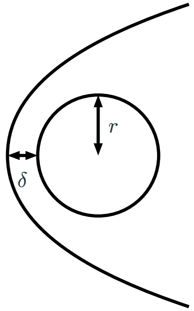
Deceleration





- Calculate the free-stream speed to get the same numerical shock stand-off as the experiment
- Analytic deceleration calculated based on steel and aluminium ball bearing, with a conservative estimate of $C_D = 1.6$

Conclusions



- Unable to match the observed shock stand-off
- Explored some possible explanations for the differences
  - Viscous shock layer interactions ❌
  - Flow contamination ❌
  - Deceleration ❓
- Not enough information in the paper to calculate deceleration (e.g. material of bearing, or pressure for each shot)
- Not enough information for validation of CFD codes