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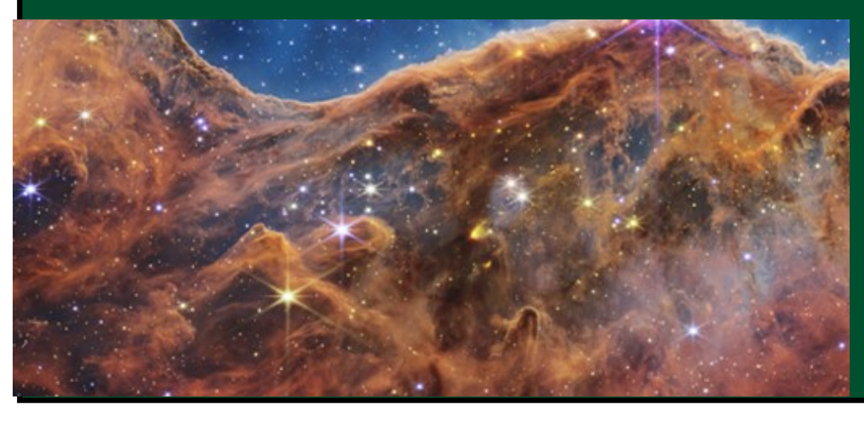

A Universal Design Optimisation Framework for Chemical Sensing Apparatus in Supersonic Flows

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1. Introduction

The Interstellar media is a **low temperature** (<100K) vacuum, comprised of gas and dust. The ISM contains upwards of **450 species** have which are involved in **6000+ gas phase** reactions. Some reactions have been suggested to be pathways to **complex organic molecules** (COM's), potential **precursors to life**. Experimentally, low temperatures are obtained by expanding a gas through a Laval nozzle to form a supersonic jet where reactions take place. The flow is characterised using the **pitot tube method** and Rayleigh –pitot equations. Nozzles are designed using the method of characteristics (MOC) . The MOC assumes the flow is **irrotational and inviscid**, which is not representative of the actual supersonic jet as it contains a **turbulent mixing layer**, and also provides no indication of flow length. These methods are **time consuming, low fidelity and complex to set-up**, hence the use of **CFD and optimisation** could improve nozzle characterisation and future nozzle design.

2. Experimental Method

Converging Diverging Nozzle profiles for a particular temperature and bath gas are designed using MOC:

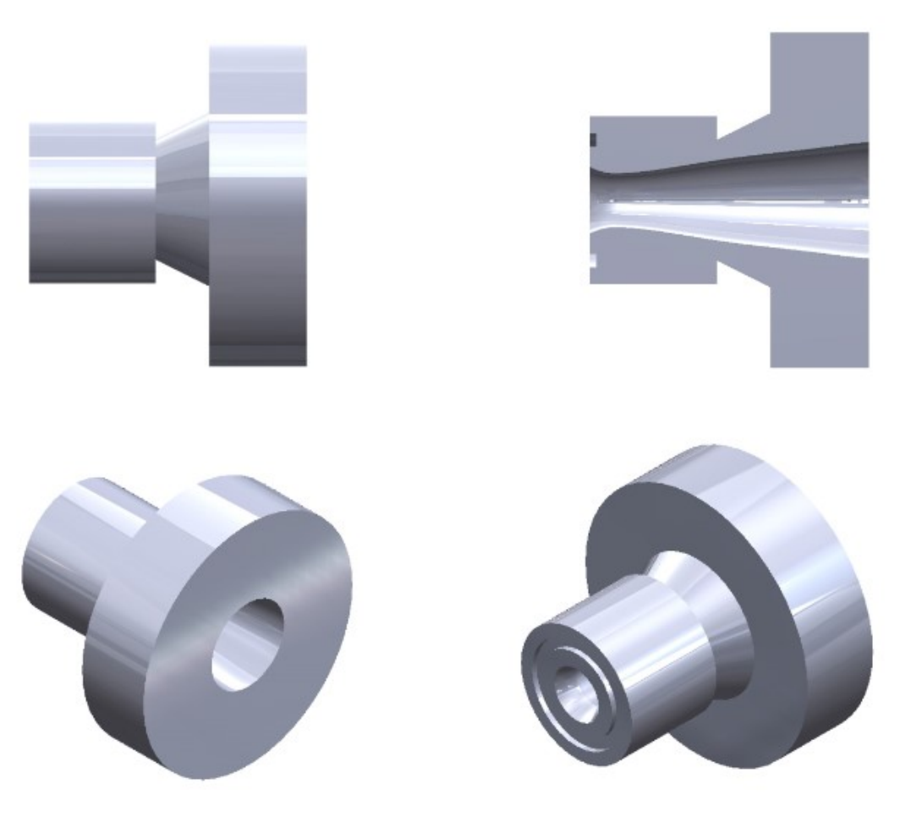
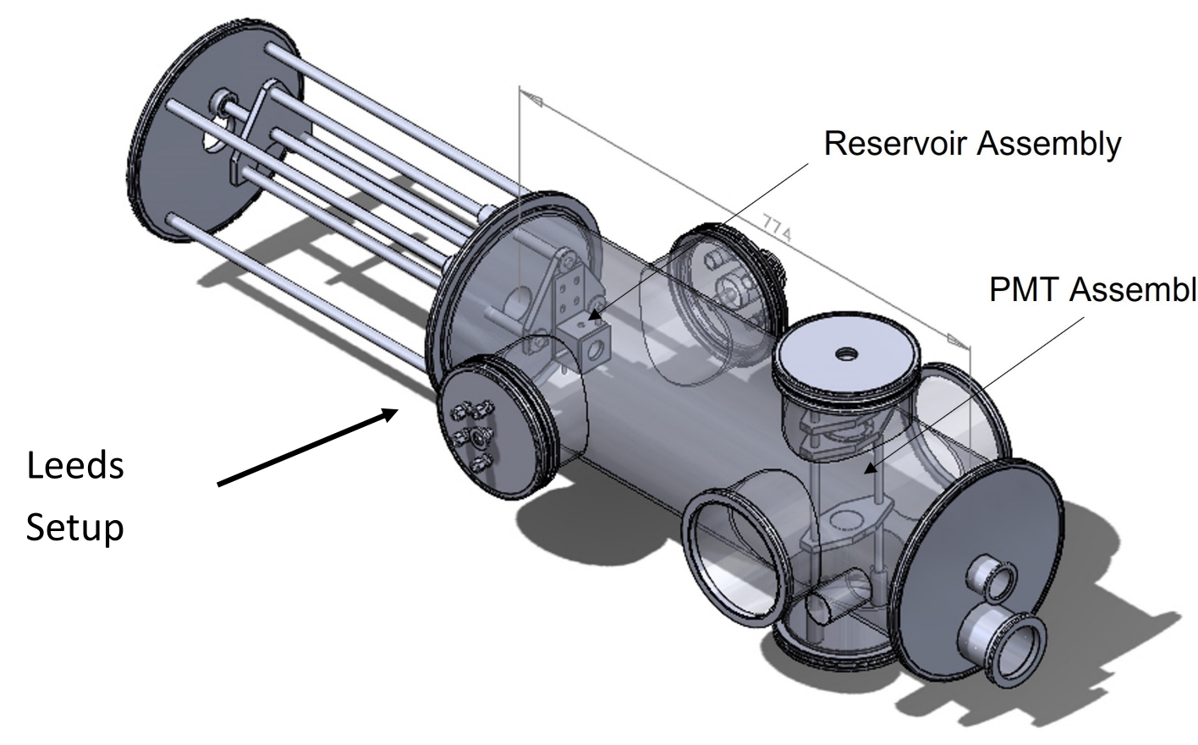
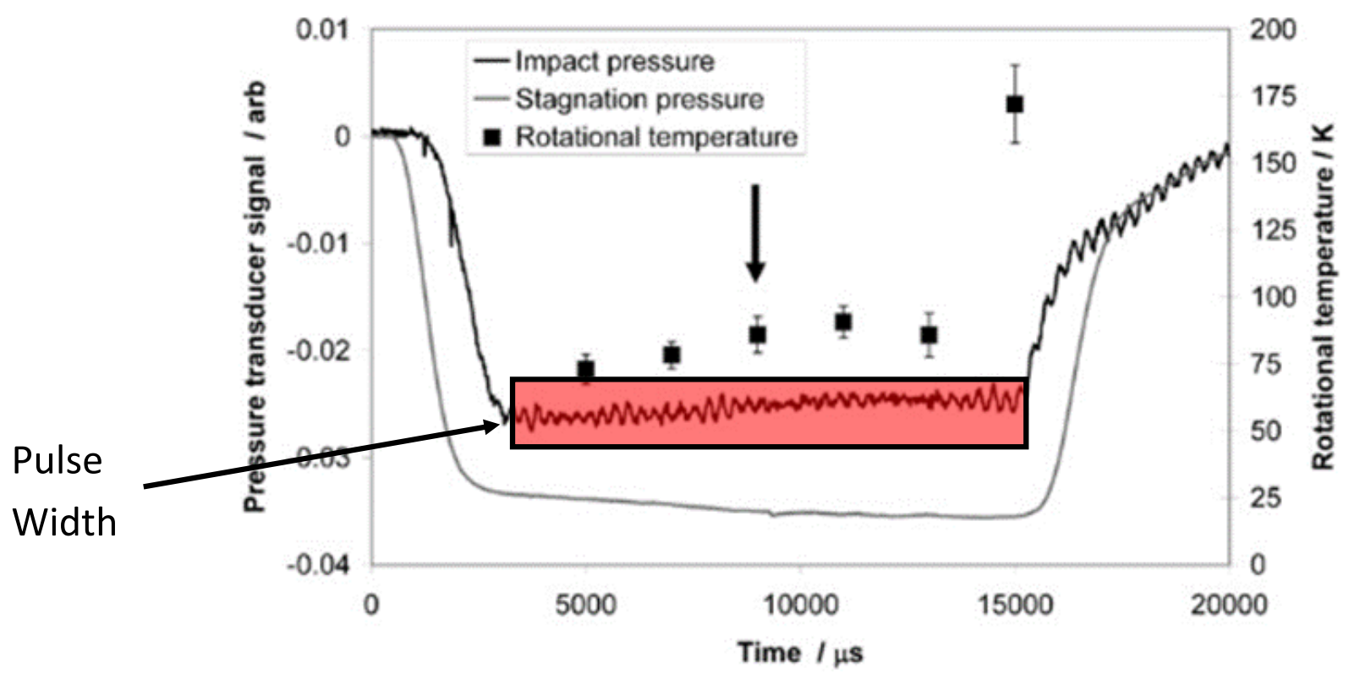


Figure 1. Mach 2.25 Nitrogen Nozzle

One nozzle and set of conditions is designed to obtain a specific temperature for reaction kinetics

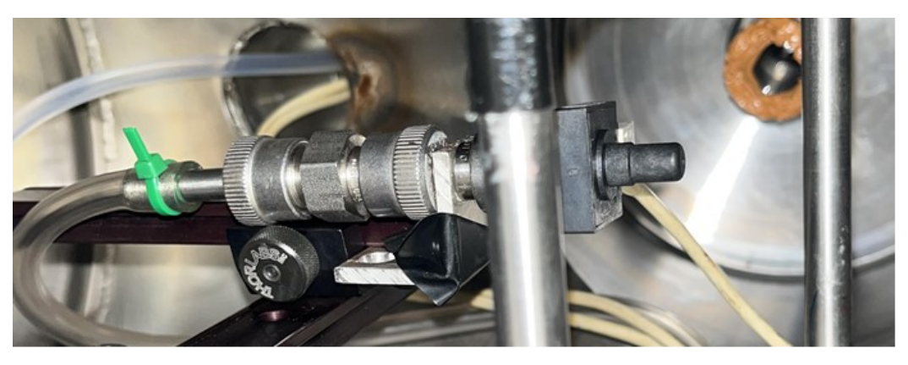
Pulsed CRESU Method is used to obtain a low temperature jet for kinetic measurements

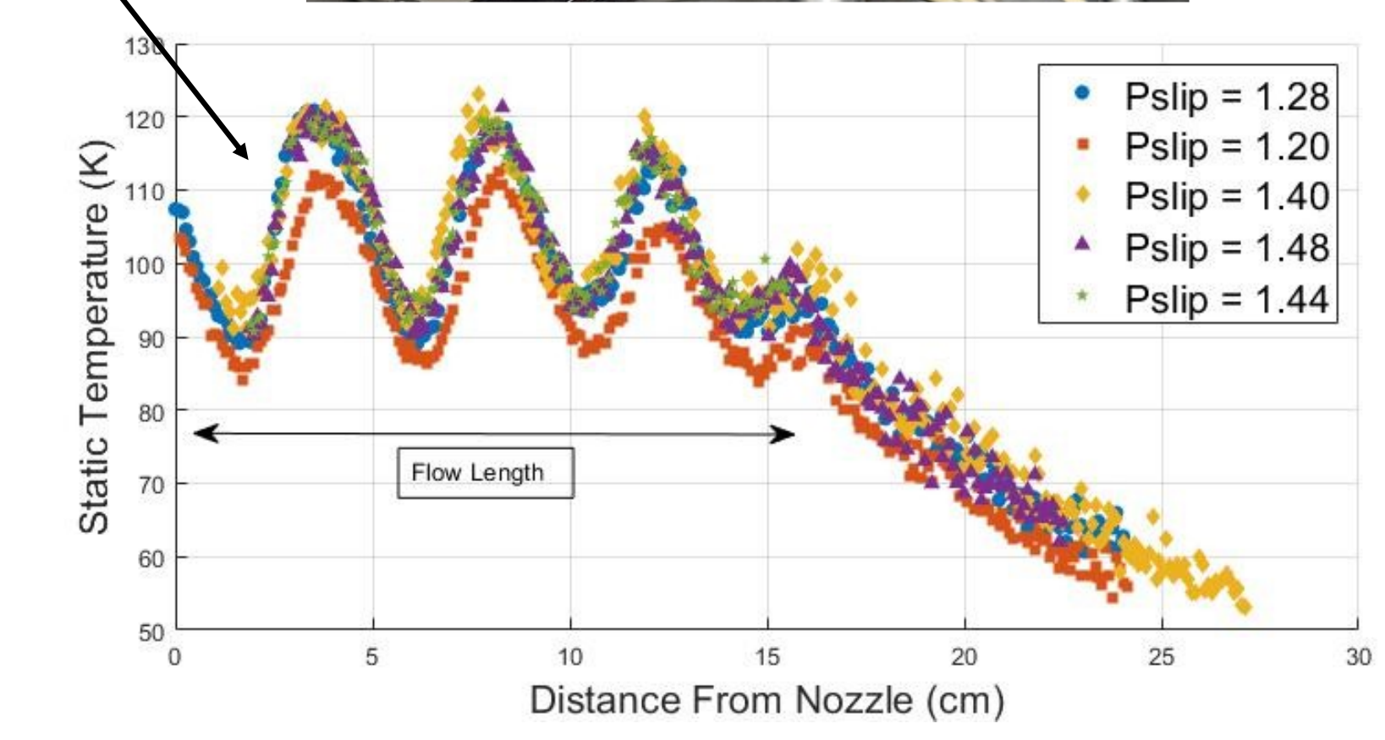




Impact pressure measurements taken using pitot tube and converted to temperature and Mach number using Rayleigh-pitot equation and adiabatic relationships:

$$\frac{P_i}{P_{\mathrm{res}}} = \left(\frac{(\gamma+1)M^2}{(\gamma-1)M^2+2}\right)^{\frac{\gamma}{\gamma-1}} \left(\frac{\gamma+1}{2\gamma M^2-\gamma+1}\right)^{\frac{1}{\gamma-1}}$$





3. Numerical Method

The Compressible Favre Averaged Navier Stokes (FANS) equations with an ideal gas equation of state and Menter k-w-SST eddy viscosity turbulence model was used to model this system.

Conservation of mass, momentum and energy:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j) = 0 \qquad \frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j}(\tilde{u}_i\bar{\rho}\tilde{u}_j) = \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\frac{\partial \bar{\rho}\tilde{E}}{\partial t} + \frac{\partial}{\partial x_j}(\tilde{u}_j\bar{\rho}\tilde{H}) = \frac{\partial}{\partial x_j}(\bar{\sigma}_{ij}\tilde{u}_i + \overline{\sigma_{ij}u_i''}) - \frac{\partial}{\partial x_j}(\bar{q}_j + c_p\overline{\rho u_j'' T''} - \tilde{u}_i\tau_{ij} + \frac{1}{2}\overline{\rho u_i'' u_i'' u_j''})$$

Scalar Transport equations for TKE (k) and specific dissipation rate (w):

$$\rho\frac{\partial k}{\partial t} + \rho\tilde{u}_j\frac{\partial k}{\partial x_j} = \tau_{ij}\frac{\partial \tilde{u}_i}{\partial x_j} - \beta^*\rho\omega k + \frac{\partial}{\partial x_j}\left[(\mu + \sigma_k\frac{\bar{\rho}k}{\omega})\frac{\partial k}{\partial x_j}\right]$$

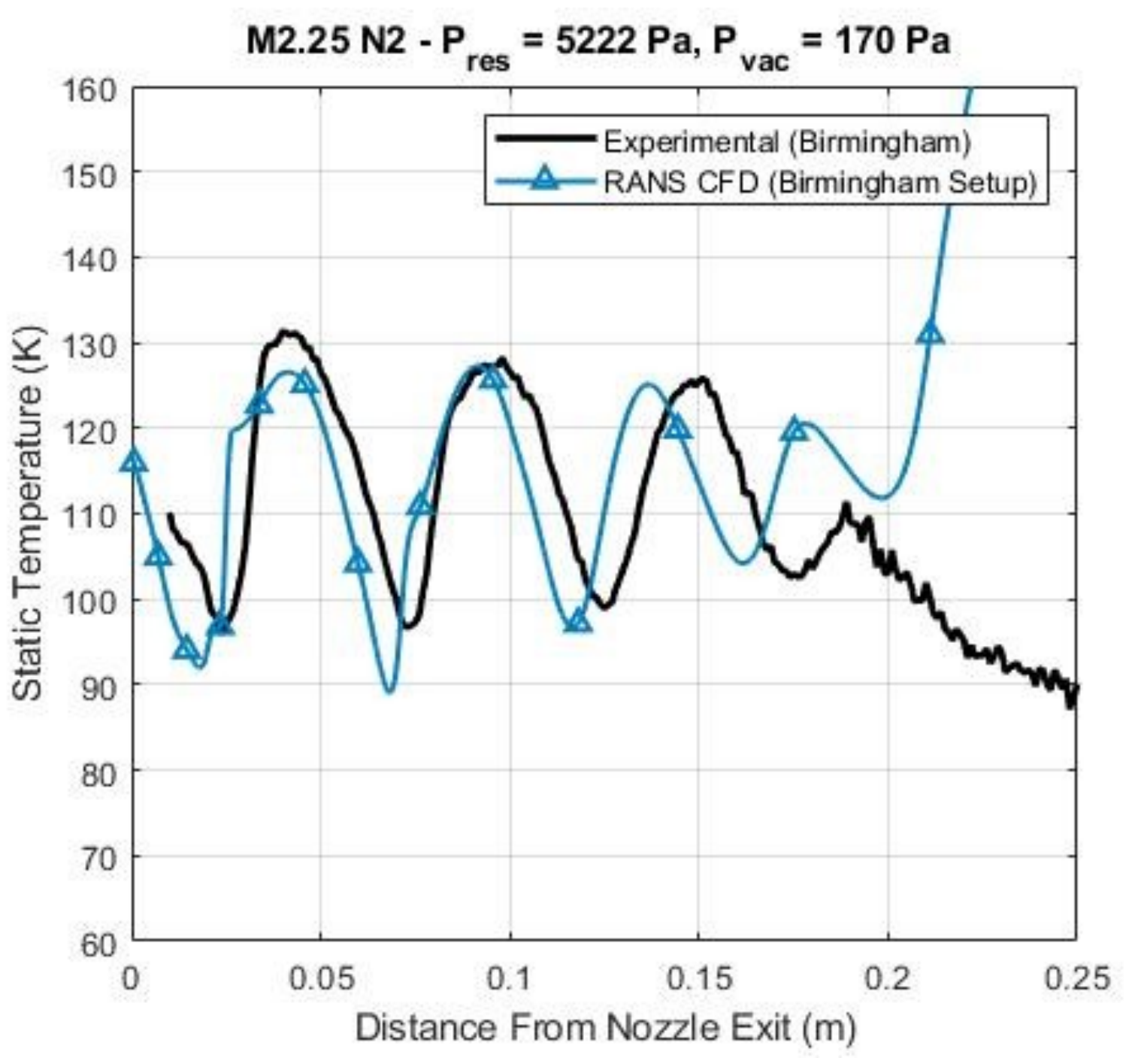
$$\rho\frac{\partial \omega}{\partial t} + \bar{\rho}\tilde{u}_j\frac{\partial \omega}{\partial x_j} = \frac{\gamma}{v_t}\tau_{ij}\frac{\partial \tilde{u}_i}{\partial x_j} - \beta\bar{\rho}\omega^2 + \frac{\partial}{\partial x_j}\left[(\mu + \mu_T\omega_\sigma)\frac{\partial \omega}{\partial x_j}\right] + 2\bar{\rho}(1-F_1)\sigma_{\omega,2}\frac{1}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}$$

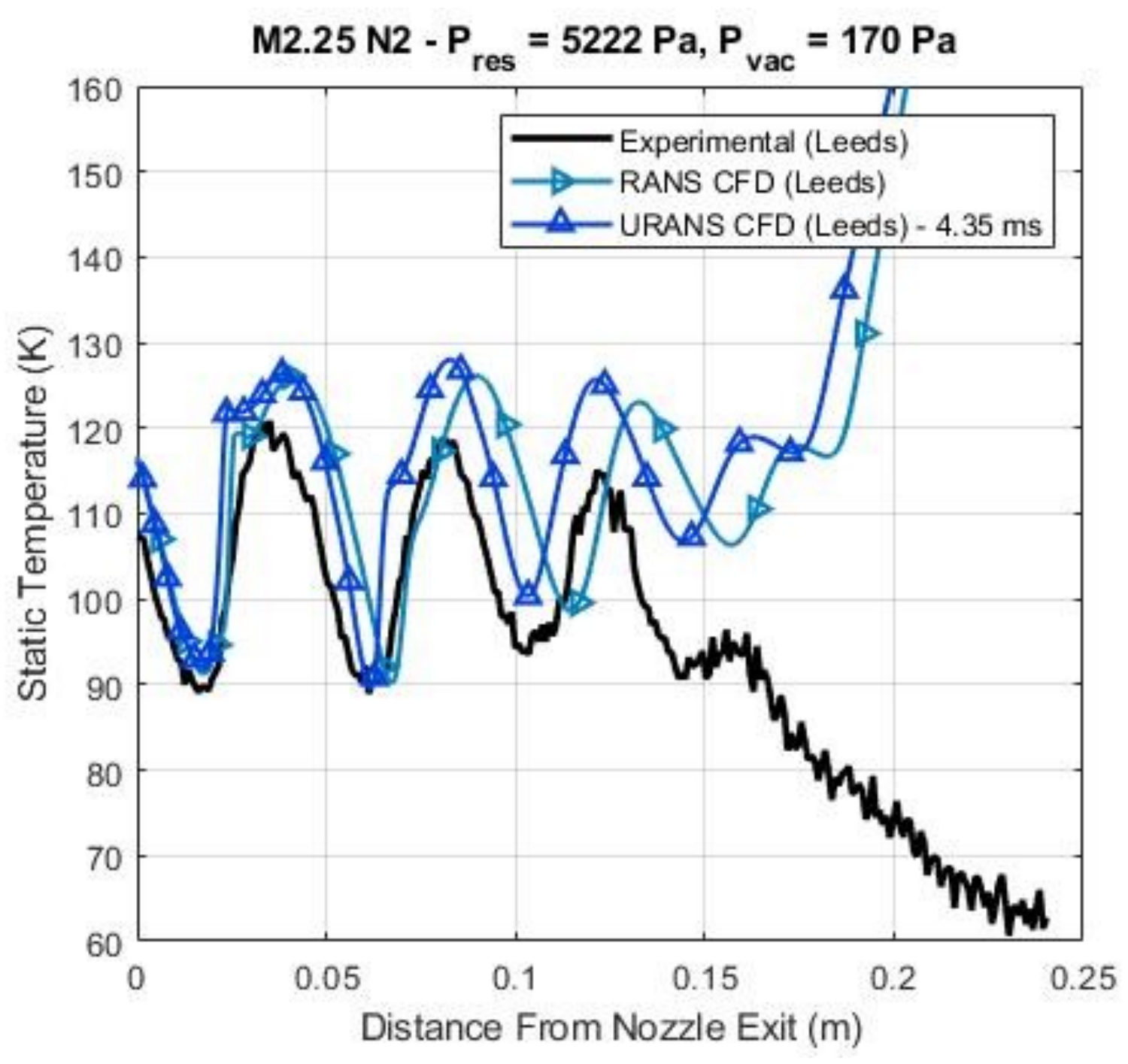
k-ω: (ϕ_1): $\sigma_{k,1} = 0.85$, $\sigma_{\omega,1} = 0.5$, $\beta_1 = 0.075$, $\beta^* = 0.09$, $\gamma_1 = \frac{\beta_1}{\beta^*} - \frac{\sigma_{\omega,1}\kappa^2}{\sqrt{\beta^*}}$, $\kappa = 0.41$, $a_1 = 0.31$

4. CFD Based Flow Characterisation Results

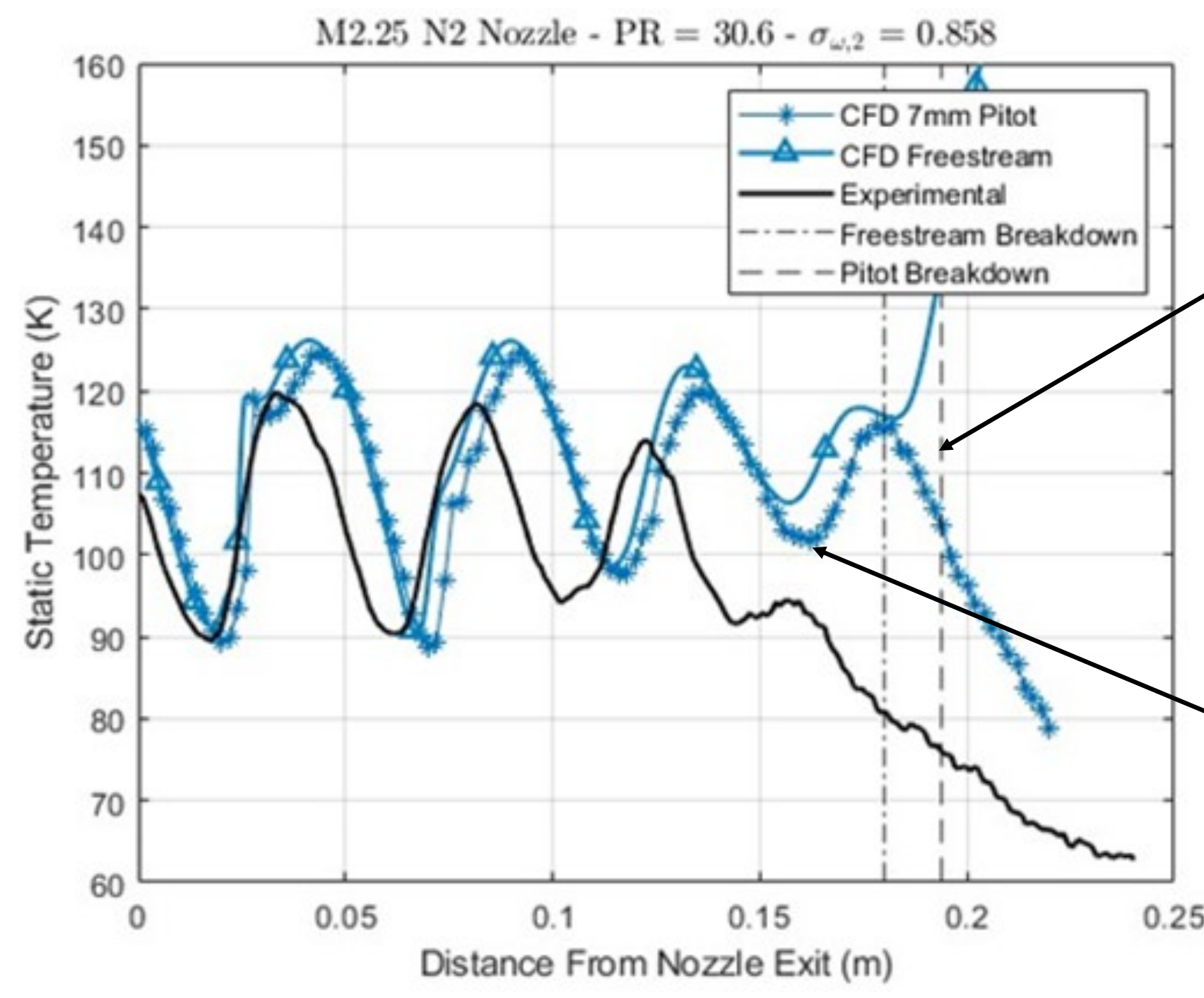
These results show comparisons between freestream CFD and experiments across the jet axis for the same nozzle and conditions with Leeds and Birmingham's CRESU setup.

Pre-expansion reservoir has a large effect on the stability and length of the supersonic jet, larger pre-expansion reservoirs approach steady state flow, whereas smaller reservoirs look to be heavily unstable and transient, which affect the quality of the jet.



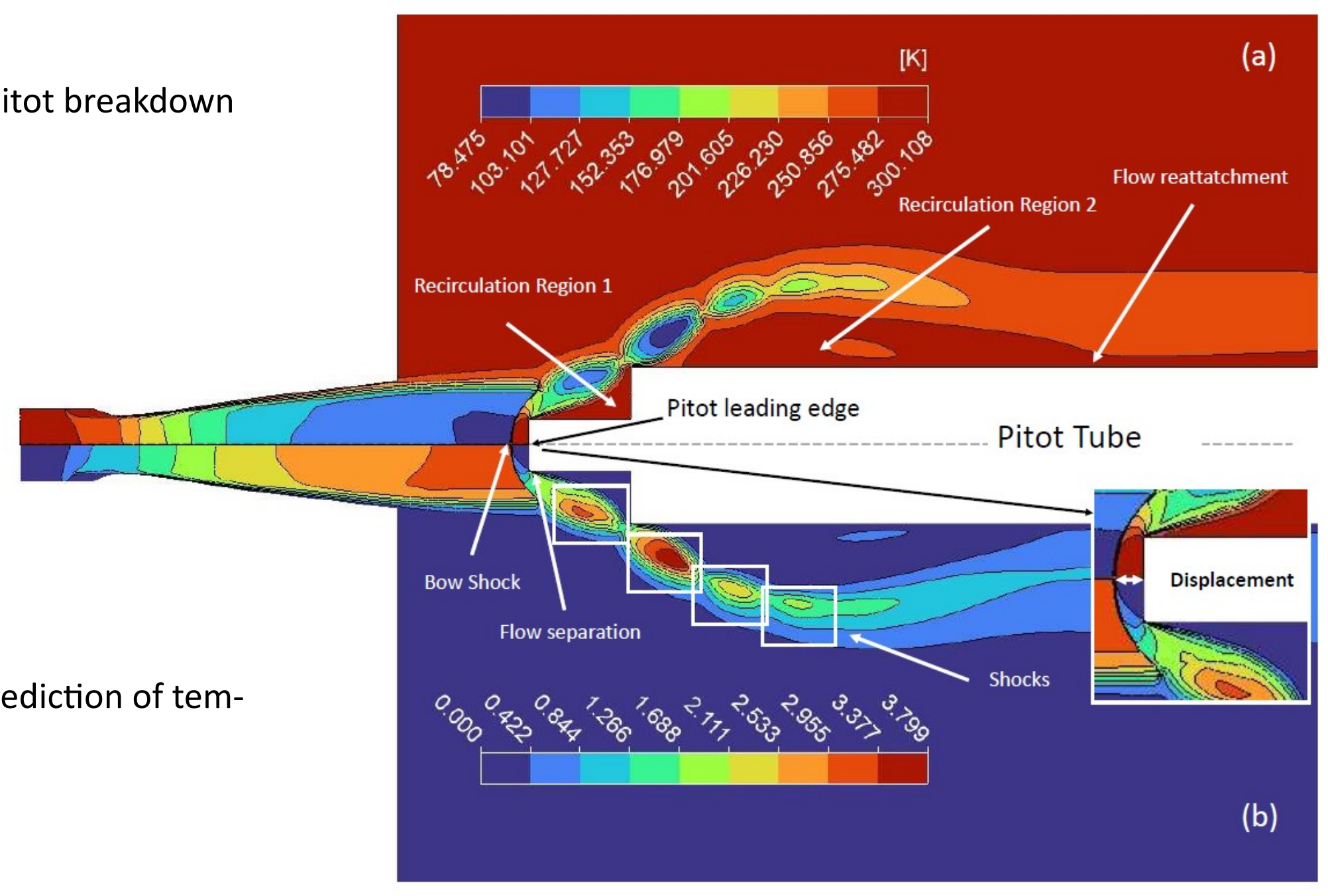


The inclusion of a pitot tube causes a phenomenon known as the displacement effect. This shifts the entire profile forward, hence this could suggest why the results at Birmingham are displaced forward in comparison to the CFD. Furthermore, the pitot tube can cause an over prediction of Mach number (under prediction of temperature), which is dependent on the pitot tube size and flow location.



Rayleigh-pitot breakdown

Under prediction of temperature

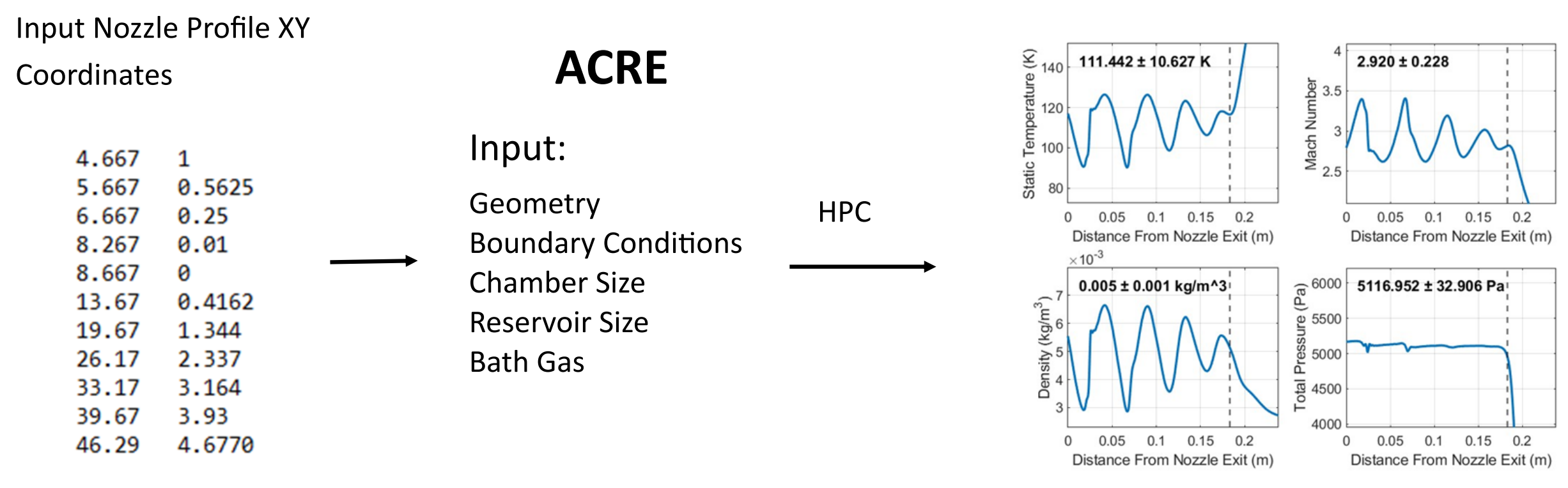


5. ACRE MATLAB Framework

ACRE Framework

(A)utomated CFD **(C)**haracterisation for Low Temperature **(Re)**action Kinetics

- **MATLAB toolbox was developed that automates the CFD workflow**, i.e. Geometry, Meshing and Solution. It allows the user to input any nozzle profile, pressure, temperature, bath gas, reservoir size and chamber size.



Input Nozzle Profile XY Coordinates

4.667	1
5.667	0.5625
6.667	0.25
8.267	0.01
8.667	0
13.67	0.4162
19.67	1.344
26.17	2.337
33.17	3.164
39.67	3.93
46.29	4.6770

ACRE

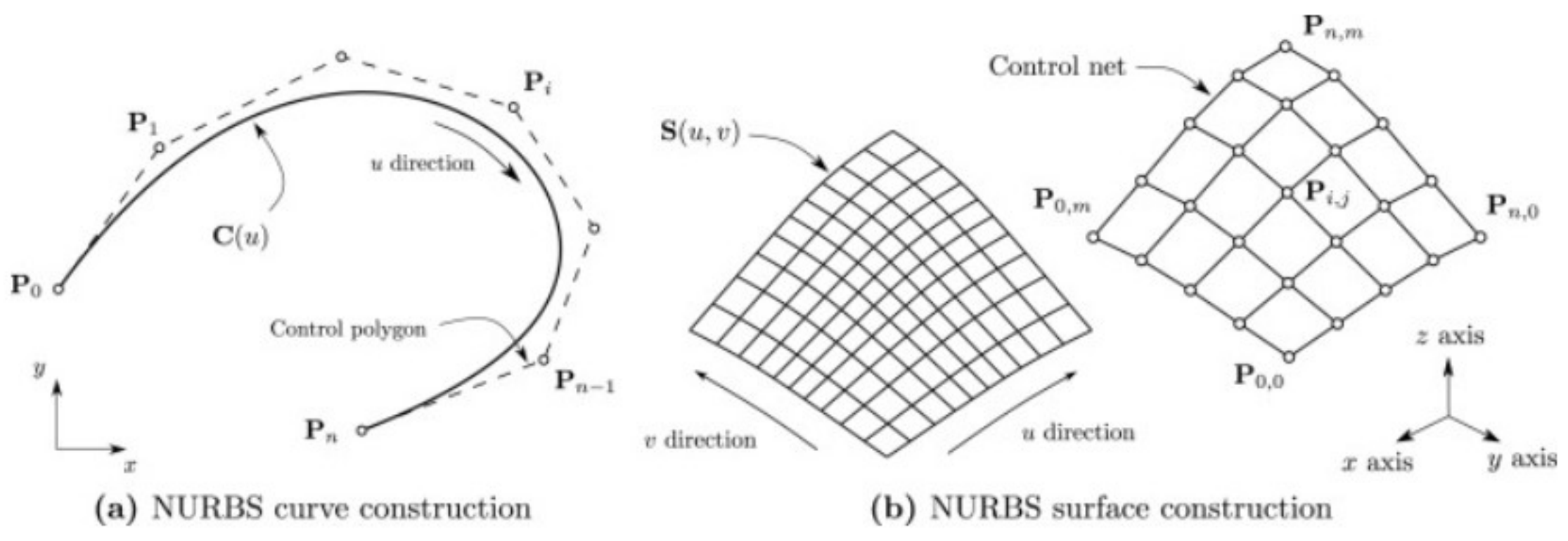
Input:

Geometry
Boundary Conditions
Chamber Size
Reservoir Size
Bath Gas

HPC

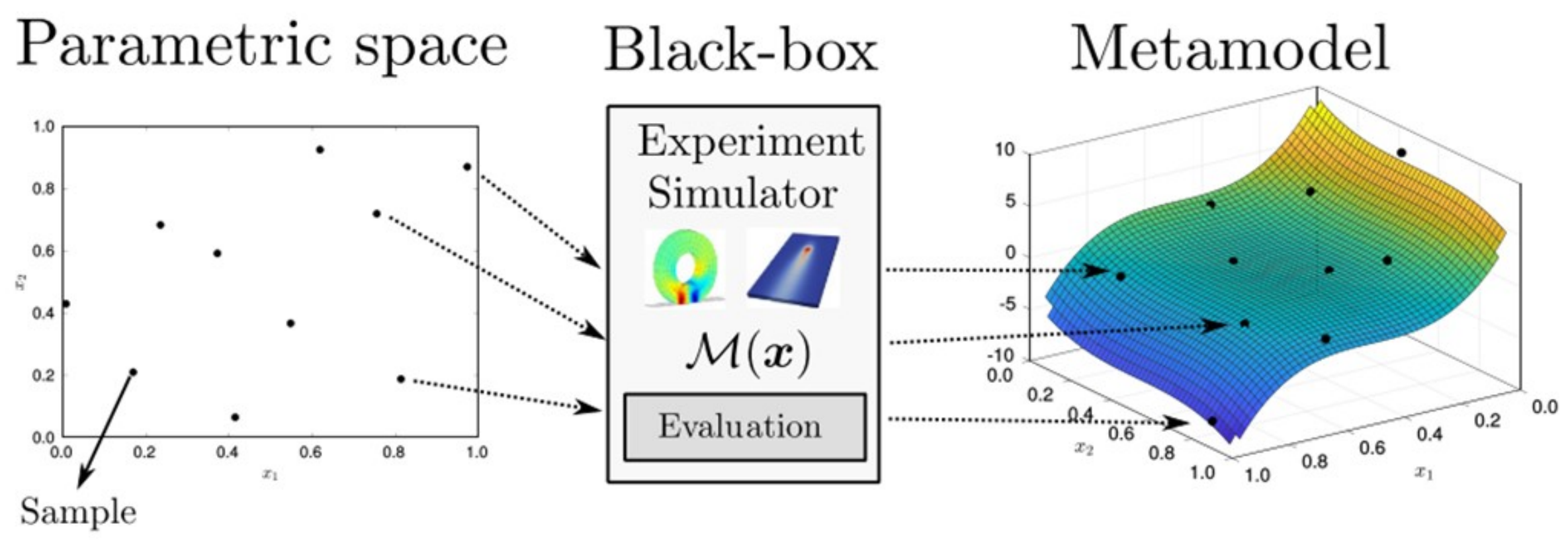
6. Future Work—Design Optimisation

Design Optimisation will be applied to the CD nozzle, where the objective function will be to minimise the oscillations in the flow and to maximise flow length. The nozzle geometry will be controlled using a freeform approach, using NURBS, which is commonly used in the aerospace industry:



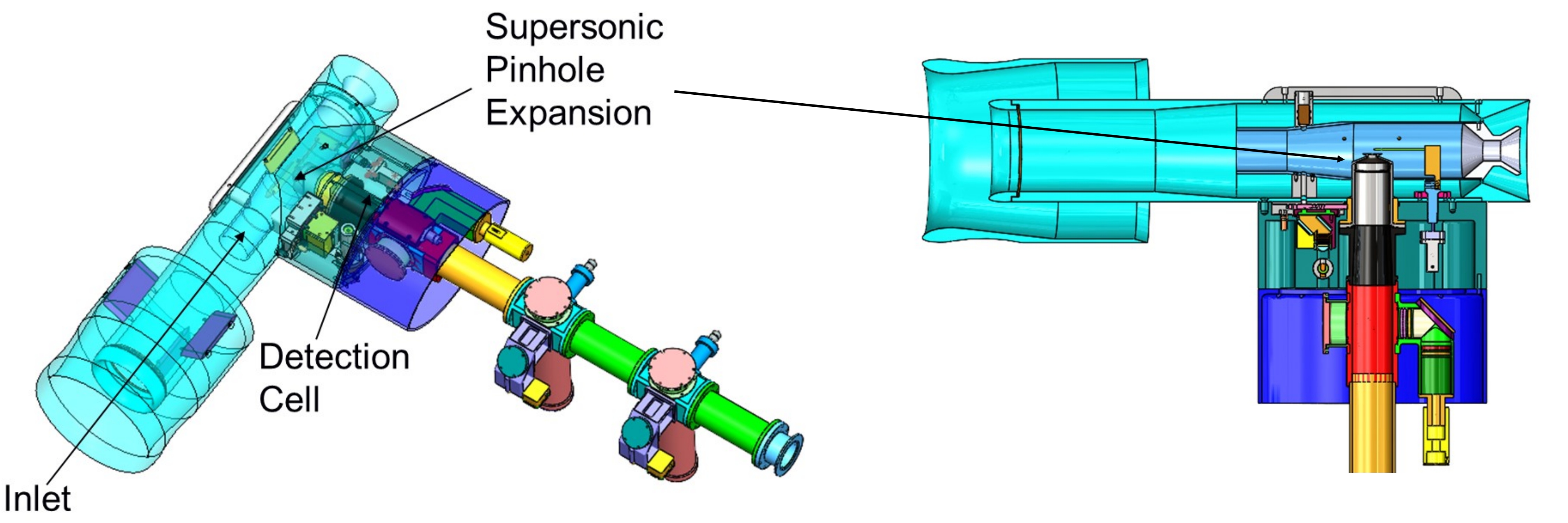
(a) NURBS curve construction (b) NURBS surface construction

As CFD calculations can be come computationally expensive, metamodels are often used as a cost-effective approach to model a complex system:



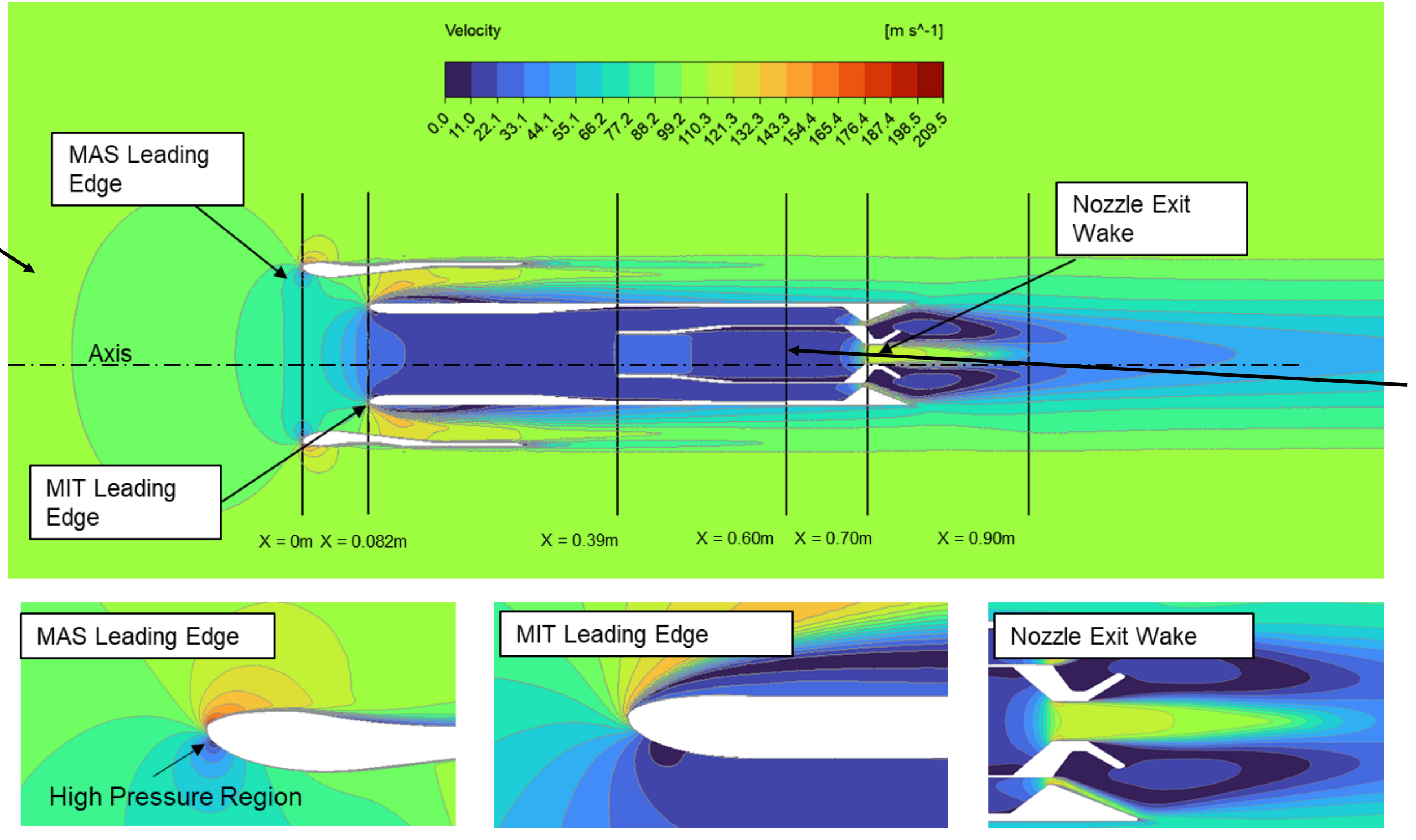
Once the metamodel is obtained, an optimiser can be applied to obtain the optimal design based on the objective functions.

7. Other Application Areas (Atmospheric Measurements using FAGE)



External flow model excluding Pinole region, showing velocity reduction across the device

~ 5.81 reduction in velocity



We want to know how we can optimise the shape of this to maximise velocity reduction in he pinhole region.