ACRE User Guide

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12th June 2024

1 Background

The CRESU method is used to experimentally obtain rate constants for low temperature gas phase reactions that occur in both planetary atmosphere and the interstellar media. The CRESU method at its core, uses a converging diverging (Laval nozzle) to generate a low temperature jet. The characteristics of the jet are determined by the bath gas (Helium, Argon or Nitrogen), reservoir pressure, vacuum chamber pressure and the shape of the nozzle profile. CD Nozzles have always been designed using the Method of Characteristics, which is an analytical way to solve the compressible potential equations. The solution to this process is a shock free nozzle that creating a downstream jet of one particular temperature. As the MOC assumes and inviscid flow, an analytical relation to calculate the boundary layer thickness across the nozzle profile is added to the profile.

The MOC does not give any insight into (i) the length of the flow, which is controlled by the downstream development of the turbulent boundary layer that surrounds the stable core region, this determines both the residence time of the reaction species in the jet and what reactions can be performed and (ii) the magnitude of the shock structures which cause variations in the jet temperature. This is important as large variations in jet temperature contribute to errors in the kinetic rate constants that are measured. Fundamentally this method requires the designed nozzle to be manufactured and tested before its true performance can be determined. It is also very common that a nozzle designed using the MOC doesn't predict as expected and many attempts have to be made to design a quality nozzle for a particular temperature.

Therefore the ACRE framework was developed to provide an accessible, high fidelity tool that can be used to accurately predict low density, high mach number converging diverging nozzle jet characteristics in the pulsed CRESU method.

2 ACRE Framework

2.1 User Defined Inputs

ACRE is a MATLAB toolbox that was developed to be used on a Linux system. It uses MATLAB to automatically generate Ansys scripts subject to a large set of user defined inputs. A high-level overview of the workflow ACRE uses is shown in Figure 1. The user inputs as shown in the bullet points below, but user are able to change all parameters of interest, which includes the nozzle geometry, reservoir pressure, vacuum pressure, reservoir and chamber geometry. This allows the framework to be easily adapted to the setup of any CRESU group that wants to use this toolbox for CFD calculations. Note that as the code is open-source, the scripts can be adjusted or replaced with others to mimic other CRESU setup's, such as the continuous systems, which require the inlet boundary to be moved.

- Boundary Conditions - Reservoir Pressure (P_{in}), Vacuum Pressure (P_{out}) and Temperature (T_{in} and T_{out})
- Bath Gas - Limited to Nitrogen, Helium and Argon
- Nozzle Geometry (Requires XY coordinates and has to be Axisymmetric)
- Chamber Length ($L_{chamber}$) and Chamber Radius ($r_{chamber}$)
- Reservoir Length (L_{res}) and Chamber Radius (r_{res})

- Inlet Diameter (d_{inlet})
- Outlet Position (L_{outlet}) and Outlet Diameter (d_{outlet})
- Number of CFD iterations (This is set to 1000 at default for pressure based and 5000 for density based).
- Pseudo time scale factor (Increasing this increases rate of convergence although may cause stability issues. Decreasing improves stability but takes longer for the solution to converge).
- Number of CPU cores to use to solve the CFD calculation
- Ansys version to use (2021R2, 2022R1 or 2023R1).
- Mesh density can be changed by a user defined factor.

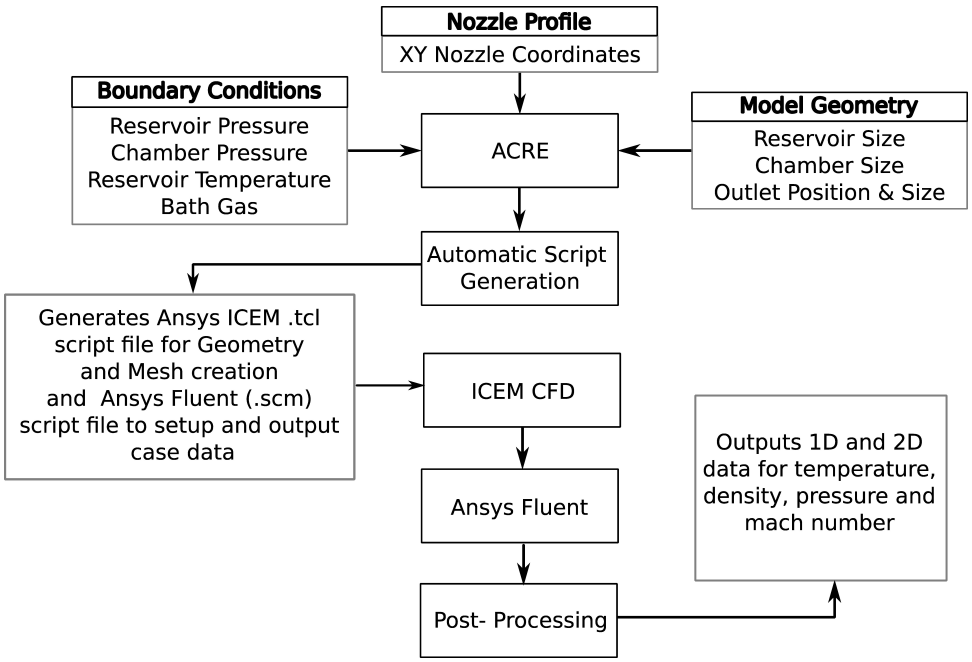

Figure 1: High level overview of the ACRE framework. The main MATLAB script automatically generates script files for Ansys Fluent and Ansys ICEM and automatically runs these scripts with the appropriate software. The data is then outputted from the CFD simulation and post-processed to allow the user to view the 1D and 2D data of their supersonic nozzle flow.

2.2 Software Requirements

To run this on a Linux based HPC system the following software is required:

- MATLAB 2022 or later
- Ansys Fluent 2022 or later
- Ansys ICEM 2022 or later

The minimum hardware requirements to run ACRE is a 4 core CPU with 16GB of RAM. Although it is recommended that 20-40 cores are used on a HPC to exponentially speed up calculations.

2.3 Geometry and Modelling Setup

The geometry is used in the CFD is shown in Figure 1 with the main characterising dimensions. These relate to the ones used in the CRESU method and should be applied to suit your specific case. The geometry is modelled in such a way that the nozzle is located at one end of the vaccum chamber. The chamber size can be made smaller to reduce computational costs although ensure that the results are independent of this. The following modelling numerical approach is used for low temperature, low density supersonic flow:

1. Steady state coupled pressure based finite volume solver, The supersonic jet reaches steady state before pitot and kinetic measurements are made.
2. Second order discretisation schemes
3. 2D axisymmetric domain, inlet and outlet are modelled as an annulus (although these has negligable effect on results). The flow is rotational invariant.
4. Favre-averaged Navier Stokes (FANS) with the k-ω-SST turbulence model with viscous heating and ignoring compressbility effects.
5. Equation of state is ideal gas as nobles gasses are ideal
6. Viscosity, specific heat capacity and thermal conductivity are dependent on temperature.
7. Calculation is initialised with full multi grid (FMG) initialisation to speed up convergence.
8. ACRE is currently limited to Mach < 5

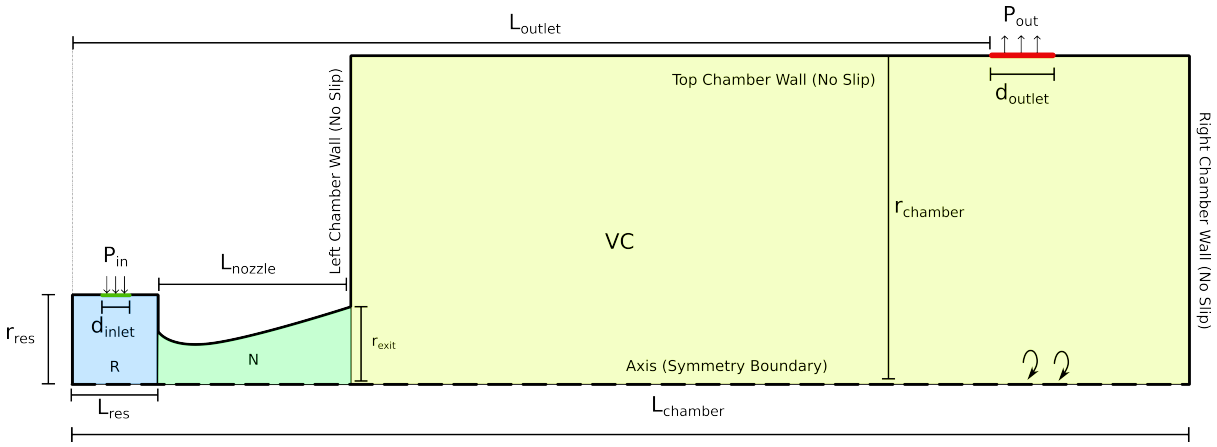

Figure 2: Schematic of geometry used in ACRE CFD framework.

2.3.1 Meshing

The mesh for every case that you run will look very similar to Figure 3. In this, the elements are quadrilaterals and aligned with the flow direction. The elements generally an aspect ratio ≈ 1 in the wake region and excellent orthogonality. Having these features in a mesh greatly increases the accuracy for large gradient flows, the speed of calculation and rate of convergence.

The meshing script is setup in a way where the mesh adapts to your particular nozzle geometry. Therefore if you use a larger nozzle, the number of cells will increase and the mesh density will stay the same. The framework also allows the user to change the global mesh density by any factor they would like. This gives the user more control, and can be used to perform a mesh dependence study if a factor of 0.5, 1 and 2 is used. This will mimic a grid convergence study with a refinement ratio of 2. ACRE also gives the user the ability to change the first layer height on the nozzle wall, which is used to resolve the boundary layer. These features have been completely detached from the CFD workflow, and only need to be set in the main code within MATLAB.

Setting the mesh factor to 1 uses the default mesh density settings. This mesh has been tested on a Mach 3 and Mach 4 nozzle, and has been shown to have mesh independence for both cases using this mesh. If you intend to go higher than Mach 5 for testing purposes, you may want to increase this mesh factor and perform your own mesh dependence tests for peace of mind.

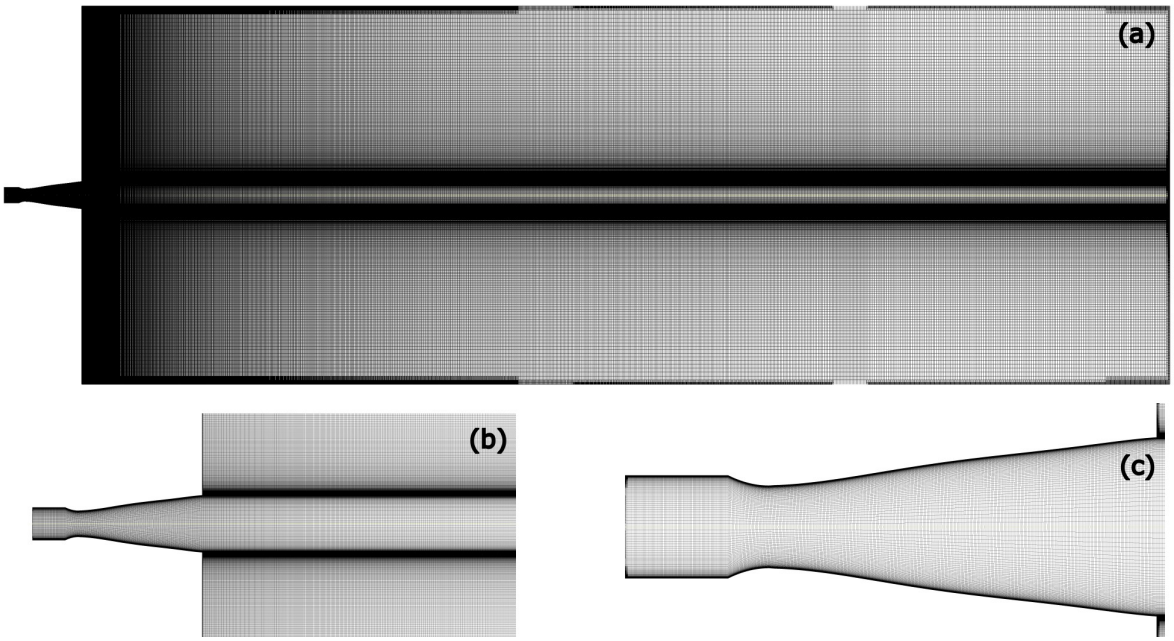

Figure 3: Picture of Meshing approach used for supersonic nozzle flow. Note that cells are clustered towards the walls to resolve the boundary layer and flow separation which is cruitial in predicting jet structures.

3 Using the ACRE Framework

3.1 Making the Toolbox Compatible with your System

Once you have successfully downloaded the framework and uploaded it to your Linux based HPC, you need to go through the following steps to make sure ACRE is compatible with your system.

1. Open up the MATLAB script named "cfd_blackbox.m".
2. Within this code, you need to find the 6 lines (Located between lines 244 - 255 and 293 to 302) that look like the following

   ```
   /apps/applications/ansys/2023R1/1/default/v212/icemcfd/linux64_amd/icemcfd/
   output-interfaces/fluent6 -dom $script_dir/Meshing/project1.uns -b
   $script_dir/Meshing/project1.fbc -dim2d $script_dir/' Solution_Folder '/Mesh']);
   ```

3. Currently the directory used for the meshing script is set to the directory on the Leeds HPC. It calls fluent6 from the Ansys directory to save project.uns. This directory is currently:

   ```
   /apps/applications/ansys/2023R1/1/default/v212/icemcfd/
   linux64_amd/icemcfd/output-interfaces/fluent6
   ```

4. You need to locate where the fluent6 file is on your HPC (you can do this by going through the directories). It will be similar to the one in this example. Once you are in the directory that contains fluent6, you can type 'pwd' and get the file path of this folder.
5. You need to edit the fluent6 directory to match your system. Do this for all version of Fluent (if you have them).
6. Once this is done you can close "cfd_blackbox.m" and you don't need to access the file again if you don't want to add your own features.

3.2 File Structure and Information

When you download ACRE onto your HPC, you should have the following files and folders as shown in Table 1. Don't worry if you don't have the Meshing folder as the MATLAB script will make this for you when you start running your own simulations. There are also folders in this directory containing studies that were performed to show that the meshes used for the numerical simulations are mesh independent. It also shows a study comparing the two solvers, both density and pressure based. There is also a benchmark case on the M2.25 nozzle (profile found in /Example_Nozzle) so you can perform a test study and ensure that ACRE is working properly by comparing your resutls with this case.

Folder/File Name	Information
/Example_Nozzles	Contains the 1D XY coordinates of various nozzle profiles that are available at Leeds.
ACRE_ARC4 _run.sh	Example script to run the framework on the Leeds HPC
cfd_blackbox.m	Main code that is used to interact with Ansys to generate the geometry, mesh, and solution files.
CFD_Macro.scm	This is the CFD script used to automatically setup the CFD case using the pressure based solver.
CFD_Macro_DBS.scm	This is the CFD script used to automatically setup the CFD case using the density based solver.
GeoMesh_Macro_Linux.tcl	This is the script that gets generated automatically and is used in ICEM to generate the mesh and geometry for the case at Leeds (where the nozzle is the same radius as the reservoir).
GeoMesh_Macro_Linux_2.tcl	This is the script that gets generated automatically and is used in ICEM to generate the mesh and geometry for the case at Birmingham (where the nozzle is smaller than the reservoir).
MATLAB_Output.txt	Contains the output from MATLAB, mostly used as a debugging tool
nozzle_profile.txt	Contains the 1D XY nozzle profile of interest (user input)
nozzle_profile_formatter.m	This Is a script that formats the XY coordinates of the "nozzle_profile.txt" and outputs the formatted values into the "NozzleProfileFormatted.txt" file
Parametric_Study.m	This is the main script that will be used to interact with the cfd_blackbox. It contains the values that can be changed by the user.
ScriptChanger.m	This script is used to in the blackbox_cfd code and it changes the script files subject to what the user sets in the Parametric_Study.m file

Table 1: File structure of ACRE framework

3.3 Seting up a Study

You need to copy the XY coordinates of your nozzle into the file named "nozzle_profile.txt". The coordinates should be in mm and the format of the XY coordinates should be identical to what is seen in Figure 4. You only need the 1D axisymmetric profile of the nozzles for these numerical simulations. Note that you just need the number and not the headings. Make sure that the rows are separated by a tab. NozzleProfileFormatter will take care of formatting the coordinates for Ansys ICEM and place the nozzle inlet at x = 0. You can have as many XY points as you wish, although it is recommended to have at least 100-200 points to capture the curvature of the profile accurately. Note that the x coordinates of the points need to increase down the column or the ACRE framework will put out an error.

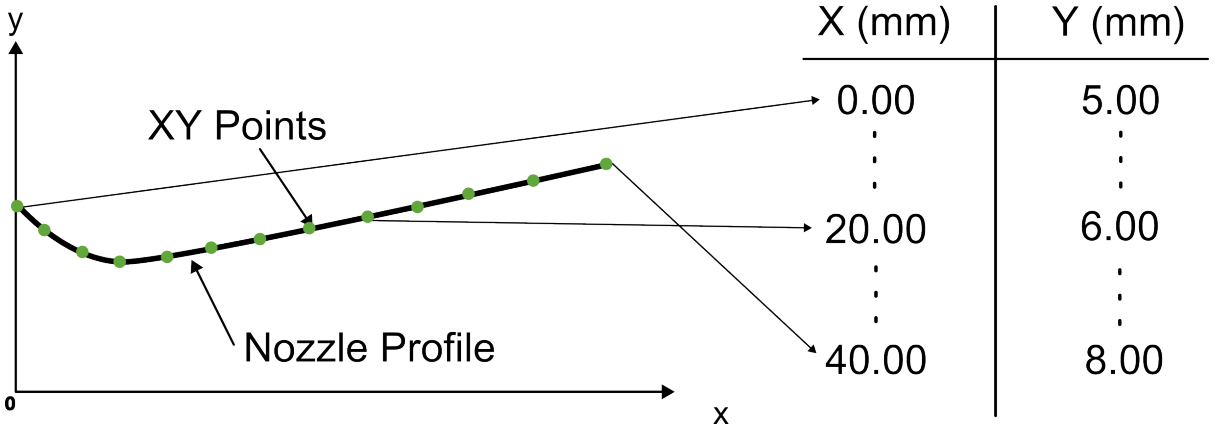

Figure 4: How to obtain XY coordinates to use in the ACRE framework. x = 0 is the axis of the nozzle.

Open you have inputted and saved the XY nozzle coordinates, open the file named Parametric_Study.m. Here you will find the input values for the cfd_blackbox code. In no particular order, these are shown in Table 2. You will need to change all these variables to match your particular setting. There have been various CFD-associated parameters added for you to play around with, such as mesh density, and solver type. In the parametric_study.m script you will find that you can input a combination of reservoir pressures, chamber pressure and run names. These are the following lines:

```
Pin = [4900 4950 5000 5050 5100 5150];
Pout = [170 170 170 170 170 170];
Solution_Folder = {'Run1', 'Run2', 'Run3', 'Run4', 'Run5', 'Run6'};
```

The code above is set to run six cases of varying reservoir pressure with the nozzle profile you inputted in the nozzle_profile.txt file. Results from each variation will be saved in a different folder denoted 'Run1' , 'Run2' etc. You can run as many as you want, but you need to ensure that you follow the formatting above and that the number of reservoir pressures equals the number of chamber pressures and number of folders. For example, if you wanted to run 3 cases you would use:

```
Pin = [4900 4950 5000];
Pout = [170 170 170];
Solution_Folder = {'Run1', 'Run2', 'Run3'};
```

If you wanted to run one single case with a specific set of pressure conditions you would use :

```
Pin = [4900];
Pout = [170];
Solution_Folder = {'Run1'};
```

Note you can change the name of the solution folder to any string you would like, for example you could change it to:

```
Solution_Folder = {'N2_Nozzle_1_Pres_5000_Pchm_170_300K'}
```

Parameter	**Information**
CPU_Cores	Number of CPU cores you want to use to solve the CFD simulation. Make sure this number equations the number of cores in your HPC submission script
Ansys_Version	Sets the Ansys version, put 0 for 2021R2, 1 for 2022R1 and 2 for 2023R1
Tin	Reservoir Temperature (K)
Tout	Vacuum Line Temperature (K), generally always the same as Reservoir Temperature.
Pin	Reservoir Pressure (Pa)
Pout	Chamber Pressure (Pa)
Bath_Gas	Sets the Bath gas, 0 for Nitrogen, 1 for Helium and 2 for Argon
Solution_Folder	Sets the name of the folder you want your results to be in
Reactor_Length	Length of reactor in mm
Reactor_Radius	Radius of reactor in mm
Reservoir_Length	Length of reservoir in mm
Reservoir_Radius	Radius of reservoir in mm
Reservoir_Inlet_Diameter	Diameter of valve orifice that connects to the reservoir, for Leeds and Birmingham its 2.94mm.
Outlet_Diameter	Diameter ofvaccum line that evacuates gas from the chamber in mm. This makes a negligable difference when you change
Outlet_Position	Position of outlet with respect to the left most wall in mm, this makes a negligable difference when you change.
Contour	If you want to receive 2D contour data, set to this 1, if not set this to 0
Y_Sampling_Interval	This sets how far you want your contyour data away from the axis in mm. If this value is 30, you will get contour data from y = 0mm to y = 30mm in 0.03 mm intervals.
nozzle_inlet_radius	Radius of nozzle inlet you just put in the nozzle_profile.txt in mm. This is used to format your nozzle correctly.
Mesh_Density _Factor	Increases the global mesh density by this factor. The default value for this is 1, setting this to 2 will increase the number of elements by a factor of ≈ 4.
First_Cell_Height_Nozzle_Wall	Sets how close the first cell is to the nozzle wall in m. Its default value is 0.00023 (0.23mm). The y^+ value is automatically adapted although you can change this.
Solver_Type	Sets the solver type, 1 for pressure-based and 2 for density-based. Density-based requires more iterations.
$\mathrm{CFD}_{Iterations}$	This is used to increase the number of iterations, default value is 1000. Increase this for density-based solver.
Pseudo_Transient_Timescale_Factor	This is default at 0.5. Increase this to increase rate of convergence, although comes at cost of solution stability.

Table 2: Input Parameters for ACRE framework

3.4 Creating a HPC Submission script and Running ACRE

Once you are happy with the nozzle you have inputted in your nozzle_profile.txt file and you have set up the correct parameters and cases in the "Parametric_Study.m" file, you can save this file and close it.

You now need to set up a job submission script to run the framework on your HPC. There are two examples of this, which can be seen in ACRE_ARC4_run.sh and ACRE_BlueBEAR_run.sh. If you are struggling to write and submit a HPC job, you should ask your IT department for help.

In your submission script, you need to ensure that the number of cores you submit on is the same as the number of cores you set in the Parametric_Study file.

An example of a shell script that is used to submit on the Leeds HPC is shown below.

```
#!/bin/bash

#$ -cwd
#$ -l h_rt=00:30:00
#$ -l nodes=1
#$ -l h_vmem=4G

module purge
module add test ansys/2023R1
module add matlab
module add user
export ANSYSLMD_LICENSE_FILE=<License goes here>

matlab -nodisplay -batch Parametric_Study > MATLAB_Output.txt
```

The setup for your particular HPC may be different, although the main function you need to call to run ACRE is

```
matlab -nodisplay -batch Parametric_Study > MATLAB_Output.txt
```

which runs the script in batch mode and outputs information in the MATLAB console to MATLAB_Output.txt.

Note that when you download the ACRE toolbox onto your HPC, it can be run in its current state without any changes if you create a shell script and submit it to your HPC. This can be used as a reference when you test your nozzles.

The time taken for a simulation will depend on the number of cores, although on a 40-core system, it takes approximately 10-15 minutes with the M2.25 Nozzle. Using larger diameter, higher mach number nozzles with take longer. Also increasing the chamber and reservoir sizes will increase the time required to obtain a solution.

You may need to run a study to investigate the number of cores that will give you the best performance. Note that there will be diminishing returns if you throw multiple nodes (CPU's) at the problem as the data transfer between nodes causes the simulations to slow down. It is recommended that only one CPU is used for this reason.

3.5 Output Files and Data

For every run you set in the "Parametric_Study.m" file, you will receive an output folder which corresponds to the name you set in the script. So, if you set up the output folder to be 'Run1' you will have an output folder that is named Run1. In the folder, you should have received the files shown in Table 3. Note that these will be present in every solution folder you run with the ACRE framework.

If you have any questions cant fix something please feel free to contact me at scldr@leeds.ac.uk!

Folder or File	Information
/Contour_Data	This folder contains the raw data that is used to generate the data in the 2D_CFD_Data.txt file. Each file is at a different location away from the y-axis. For example 'axial_density_y_0' is the density profile when y = 0. For each subsequent file, the y value increases by 0.2mm therefore, 'axial_density_y_50' is the density profile at y = 10mm away from the axis. You don't need to look at this data, you can just look at the '2D_CFD_Data.txt' file for the 2D output.
1D_Axial_CFD_Results.txt	This contains the Mach, Temperature, Density and Pressure data across the axis of the flow (y = 0). The x coordinate in this file are formatted so that x = 0 is the position of the nozzle exit. Therefore, the negative values are the values inside the nozzle and reservoir.
1D_Characterisation.flg	MATLAB figure showing results in the 1D_Axial_CFD_Results.txt file
1D_Characterisation.jpg	JPG Image showing the results in the 1D_Axial_CFD_Results.txt file
2D_CFD_Data.txt	This contains the 2D contour data for Temperature, Mach, Pressure and Density. Like the 1D data, x = 0 means the flow at the exit of the nozzle.
axial_density, pressure, temperature, Mach	This contains the 2D contour data for Temperature, Mach, Pressure and Density. Like the 1D data, x = 0 means the flow at the exit of the nozzle.
CFD_Data.cas.h5	This is the fluent case file that was setup by the code
CFD_Data.dat.h5	This is the fluent data file that contains the CFD data of the run. You can open the case and data file if you have access to fluent to post-process if you wish.
Fluent_Output _Log.txt	Contains the output from Fluent. This will show the Ansys version, the commands used to setup the case and solution monitoring.
ICEM_Output_Log.txt	Contains the output from ICEM. This will show the commands used to setup the geometry and mesh.
Max-max-convergence.txt and Min-temp-convergence.txt	This contains the maximum Mach or minimum temperature value across the axis of the flow with each iteration. You should see that at the end of the file the values should be very similar. If they are constant, it shows the solution has converged and you can use the results.
Mesh.msh	This is the mesh file generated by ICEM (will contains lot of numbers)
Mesh_report.html	This is report generated for the mesh, it contains the number of nodes and the quality of the elements.
Variable_Output	This file contains the values that were used when you ran the case. This includes the reactor size, reservoir size, bath gas, nozzle length, nozzle radius etc. This is to allow you to double check what you inputted into Parametric_Study.m was correct.
Clock_Time_Data.txt	Contains information about how long each of the steps of the process took (geometry, meshing, solution and post-processing).

Table 3: Output Parameters for ACRE framework

4 Isentropic Nozzle Calculator

Inside the ACRE toolbox, there a folder called "Isentropic_Nozzle_Calculator". Inside you will find a variety of files. The main script in this folder is called "Nozzle_Calculations.m". In this you can put your nozzle profile of interest into the "nozzle_profile.txt" file. Ensure that the first column is the X coordinate and second is the Y coordinate. An example is already setup. The code in the main script file is "Nozzle_Calculations.m" and looks like the following:

```
Nozzle_Inlet_Radius = 5; % CHANGEME inlet radius (mm)
gamma = 1.4; %CHANGEME ratio of specific heats
Reservoir_Pressure = 5000; % CHANGEME REservoir Pressure (Pa)
Reservoir_Temperature = 300 % CHANGEME in K

AR = Area_Ratio_From_Nozzle(Nozzle_Inlet_Radius);% Calculates Area Ratio
M = Nozzle_Area_to_Mach(AR,gamma); % Calculates Mach number
PR = Pressure_Ratio_from_Mach(gamma,M);
TR = Temperature_Ratio_From_Mach(gamma,M);

disp("Area Ratio = " + AR)
disp("Mach Number= " + M)
disp("Pressure Ratio = " + PR)
disp("Reservoir Pressure (Pa) = " + Reservoir_Pressure)
disp("Nozzle Exit Pressure/Chamber Pressure (Pa) = " + Reservoir_Pressure*PR)
disp("Temperature Ratio = " + TR)
disp("Reservoir Temp (K) = " + Reservoir_Temperature)
disp("Nozzle Exit Temp/Chamber Temp (Pa) = " + Reservoir_Temperature*TR)
```

This uses the area ratio of the inputted nozzle to calculate the Mach number using the analytical 1D isentropic equation:

$$\frac{A}{A^*} = \frac{\gamma+1}{2}^{-\frac{\gamma+1}{2(\gamma-1)}} \frac{(1+\frac{\gamma-1}{2}M^2)^{\frac{\gamma+1}{2(\gamma-1)}}}{M} \tag{1}$$

where A is the local nozzle area and A^* is the nozzle throat area. The temperature, pressure and density of the flow can be determined from the Mach number using the following isentropic relationships:

$$\frac{T_2}{T_1} = (1+\frac{\gamma-1}{2}M^2)^{-1}, \tag{2}$$

$$\frac{\rho_1}{\rho_2} = (1+\frac{\gamma-1}{2}M^2)^{\frac{-1}{\gamma-1}}, \tag{3}$$

where T_2 and T_1 is the flow and inlet temperature respectively, ρ_2 and ρ_1 is the flow and inlet density respectively, and P_2 and P_1 is the flow and inlet pressure respectively. This can give a fast approximation to the nozzle exit temperature and pressure ratio required to run the nozzle at optimal conditions.

5 Example Results

Figure 5 is an example of a plots that can be made using Fluent. This shows the results from using a nitrogen nozzle from Leeds with a reservoir pressure of 5222 Pa and a chamber pressure of 170 Pa.

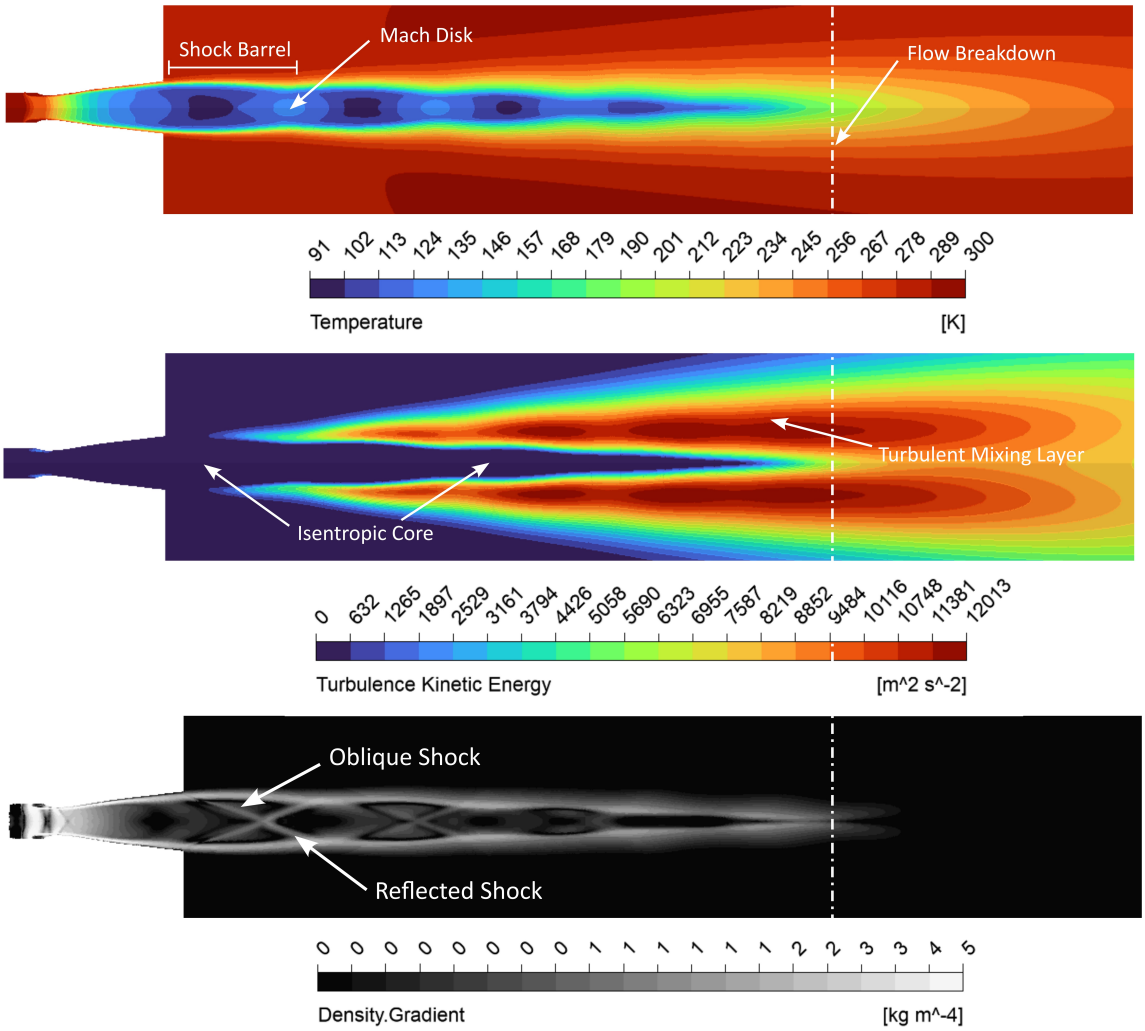

Figure 5: Freestream CFD results for M2.25 Nozzle in the Leeds setup using Nitrogen, Pres = 5222 Pa, Pchm = 170Pa and Tres = 300K. (top) Static Temperature contour with 20 contour bands (middle) Turbulent kinetic energy contour with 20 colour bands showing isentropic core (blue) and mixing layer development (bottom) numerical schlieren plot calculated using density gradient, showing expansion and compression waves that propagate from the nozzle exit. The white dotted line represents the flow breakdown (stable flow length) for the supersonic jet.

More information on the creation of the model and results from using the framework can be found in the paper titled 'Developing a Predictive Model for Low Temperature Laval Nozzles with Application in Chemical Kinetics'

If you plan to use this open source framework in your work, or you adapt it for your use case, you need to cite the original paper.