Detailed User Guide for ACRE Framework

ACRE (Automated Characterisation for Low Temperature Reaction Kinetics)

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This is a MATLAB Toolbox to be run on Linux that uses Ansys and its respective scripting languages to automate the entire CFD workflow, this includes geometry, meshing, solution setup and data output.

Users have the ability to change to change the following parameters:

- Boundary Conditions - Reservoir pressure, vacuum chamber pressure, temperature
- Bath Gas - Limited to Nitrogen, Helium and Argon at the moment
- Nozzle Geometry, a XY file of the nozzle coordinates has to be supplied.
- Chamber Geometry, the chamber length and radius can be changed.
- Reservoir Geometry, the reservoir length and radius can be changed.
- Inlet Size
- Outlet Size and Position in the reactor

The code will then take these parameters in and will alter the script files, effectively automating the entire CFD process for the user.

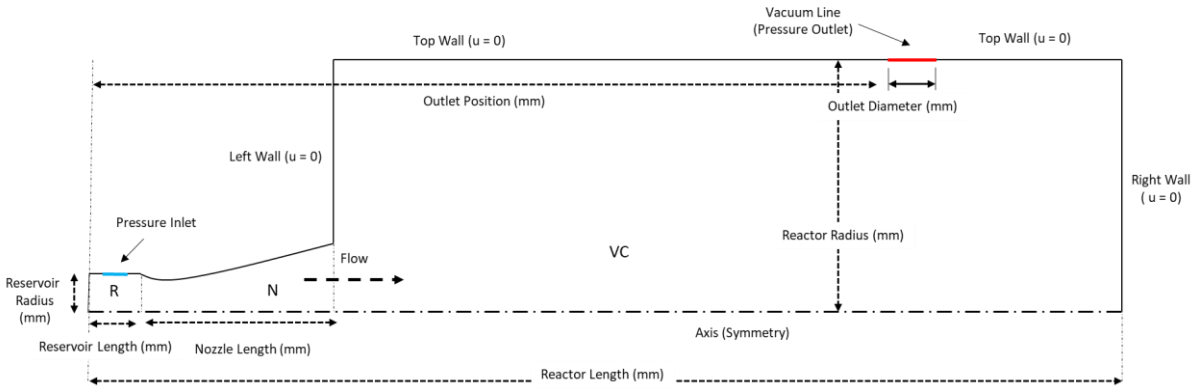
To run this on the HPC you will need:

MATLAB 2022 or newer Ansys Fluent and ICEM 2022 or newer

Brief Details of CFD Model Setup

- Steady state coupled pressure based finite volume solver.
- Second order discretisation schemes
- 2D axisymmetric domain
- Favre-averaged Navier (FANS) is used with the k-w-SST turbulence model.
- Gasses are assumed to be ideal gasses.
- Viscosity is dependent on temperature, modelling using Sutherland viscosity law.
- Currently Limited to Mach<5
- Note that the inlet and outlet are modelled as an annulus (limitation of axisymmetric)

A schematic of the computational domain used in experiments is seen below. The variables labelled here link with the ones that are set in the 'Parametric_Study.m' file discussed later in this document.



Making the Software Compatible with your HPC System

Once you have downloaded this framework and uploaded it to your HPC, you need to do the following to make sure the code is compatible with your system.

Open up the MATLAB script named “cfd_blackbox.m”. Within the script, you need to find the 6 lines, which look like the following:

```
ScriptChanger(ICEM_Script_File, 270, ['ic_exec
/apps/applications/ansys/2023R1/1/default/v212/icemcfd/linux64_amd/icemcfd/out
put-interfaces/fluent6 -dom $script_dir/Meshing/project1.uns -b
$script_dir/Meshing/project1.fbc -dim2d $script_dir/' Solution_Folder
'/Mesh']);
```

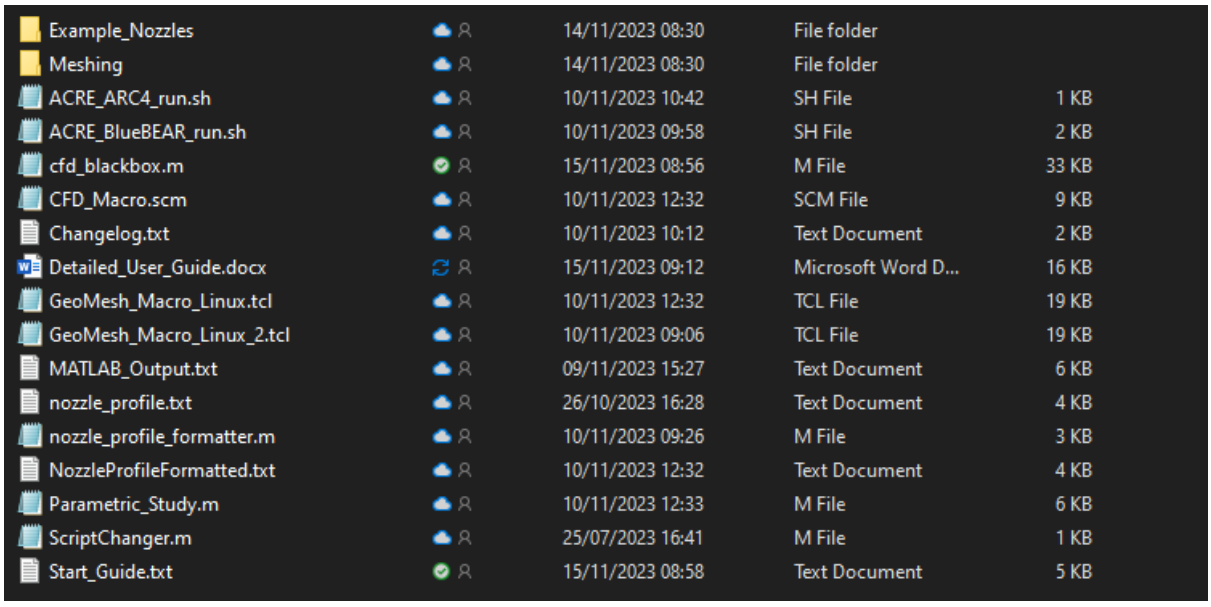
Currently this directory is set to the location of fluent6 on the Leeds HPC. You need to find this directory on your HPC and replace only this part of the code with your directory for fluent6. For example, if you want to change the directory of fluent 6 Ansys 2023R1 on BEAR you need to change the directory to:

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

Once you have done this, you can save the script and move onto running simulations!

File Structure and Information

When you download the framework onto the HPC, you should have the following files and folders. Don’t worry if you don’t have the Meshing folder as the MATLAB script will make this for you when you start running simulations.

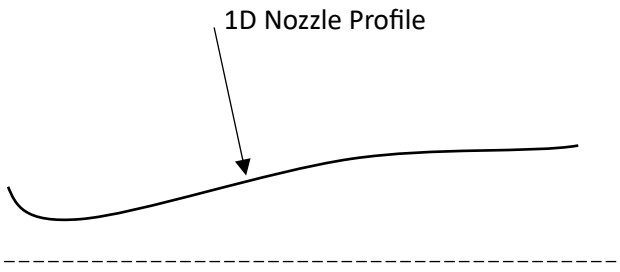


Folder/File Name	Information
Example_Nozzles	Contains the 1D XY coordinates of various nozzle profiles that are available at Leeds.

ACRE_ACR4_run.sh	Example script to run the framework on the Leeds HPC
ACRE_BlueBEAR _run.sh	Example script to run the framework on the Birmingham HPC
cfd_blackbox.m	Main code that is used to interact with Ansys to generate the geometry, mesh, and solution files. You do not need to touch anything in here except changing the fluent6 directory.
CFD_Macro.scm	This is the CFD script used to automatically setup the CFD case
Changelog.txt	Contains any updates that have been done to the framework
GeoMesh_Macro_Linux.tcl and GeoMesh_Macro_Linux_2.tcl	This is the script which automatically generates the mesh and geometry
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

Setting up a Study

Assuming you have the framework on the HPC and already have a 1D profile of a particular nozzle, you need to copy the XY coordinates of this nozzle into the file named "nozzle_profile.txt". Save this once you are finished. Make sure the X and Y coordinates are separated as seen below. You don't need to worry about the position of the nozzle in XY space, the NozzleProfileFormatter will take care of this. **You can have as many XY points as you wish.**



XY Coordinates

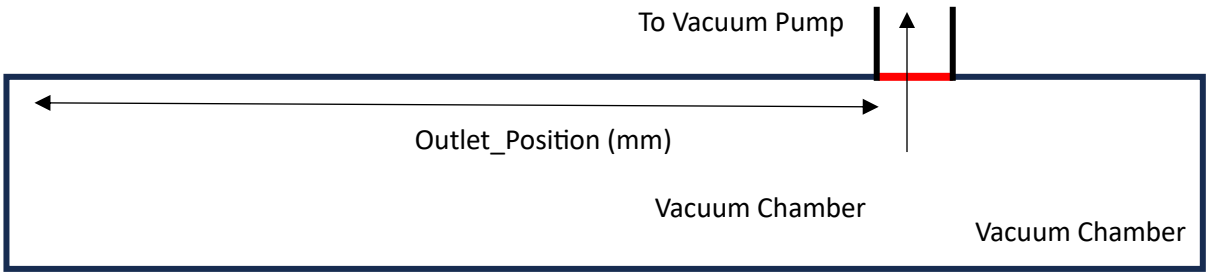
```
0.00    1
0.10    0.950625
0.20    0.9025
0.30    0.855625
0.40    0.81
0.50    0.765625
0.60    0.7225
0.70    0.680625
0.80    0.64
0.90    0.600625
1.00    0.5625
1.10    0.525625
```

Open up the file named "Parametric_Study.m", after the initial changes in "cfd_blackbox.m" this is the only file that needs to be altered. In here you will find the input values for the "cfd_blackbox.m" code. These are:

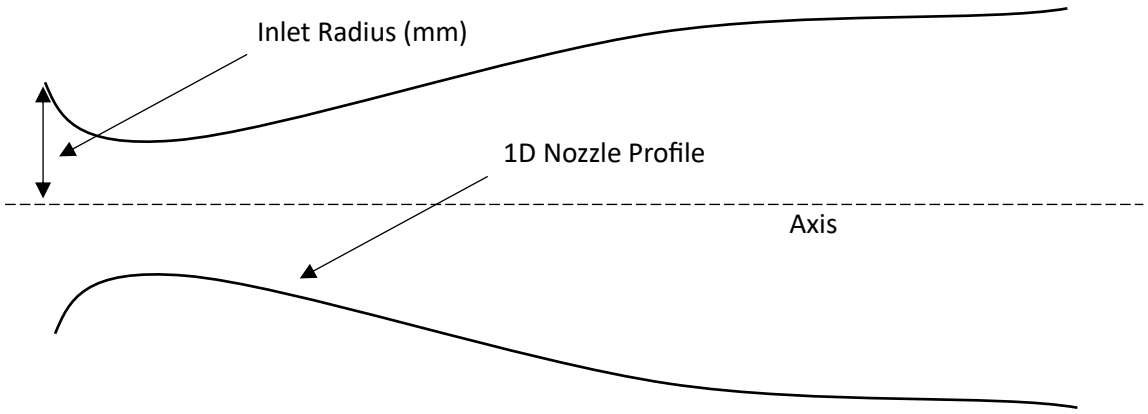
Parameter	Information
CPU_Cores	Number of CPU cores you want to use to solve the CFD simulation. Make sure this number equations the number of cores in your submission script
Ansys_Version	Sets the Ansys version, put 0 for 2021R2, 1 for 2022R1 and 2 for 2023R1
Tin	Reservoir Temperature (K)
Tout	Vacuum Line Temperature (K), should be 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	Name of the folder you want your results in
Reactor_Length	Length of reactor in mm
Reactor_Radius	Radius of reactor in mm
Reservoir_Radius	Radius of reservoir in mm
Reservoir_Length	Length of reservoir in mm
Reservoir_Inlet_Diameter	Diameter of orifice that connects the reservoir, for Leeds its 2.94mm, for Birmingham its 4mm
Outlet_Diameter	Diameter of vacuum line that evacuates gas from chamber in mm. This makes a negligible difference when you change.
Outlet_Position	Position of outlet with respect to the left most wall in mm, this make a negligible difference when you change.
Contour	If you want XY contour data, set this to 1, if not set this to 0
Y_Sampling_Interval	This sets how far you want contour data away from the axis in mm. If this value is 30, you will get contour data from y = 0mm to y = 30mm
nozzle_inlet_radius	Radius of nozzle inlet you just put in the nozzle_profile.txt in mm

Clarification on Outlet Position

Below is a simple cross sectional view of a vacuum chamber used in the CRESU experiment. The outlet position (mm) is the distance from the left wall to the edge of the vacuum line. The nozzle/reservoir in the CFD is placed at the left most side of the chamber. Therefore, the length of the vacuum chamber in the CFD is the Reactor_Length – Reservoir_Length – Nozzle_Length.



Clarification on Nozzle inlet radius



You need to change these variables to match your particular setup. If your nozzle diameter is 10 (mm), you will set 5 (mm) for the nozzle_inlet_radius. In the "Parametric_Study.m" script you will find that you can input a combination of reservoir and chamber pressures.

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 setup 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:

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

If you wanted to run one 1 case:

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

Note you can also change the name of the folders to something more fitting. For example, if you wanted the Run1 to be changed to Run1_Nozzle_1_Nitrogen you would write:

```
Pin = [4900];
    Pout = [170];
    Solution_Folder = {'Run1_Nozzle_1_Nitrogen'};
```

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

You now need to setup 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.

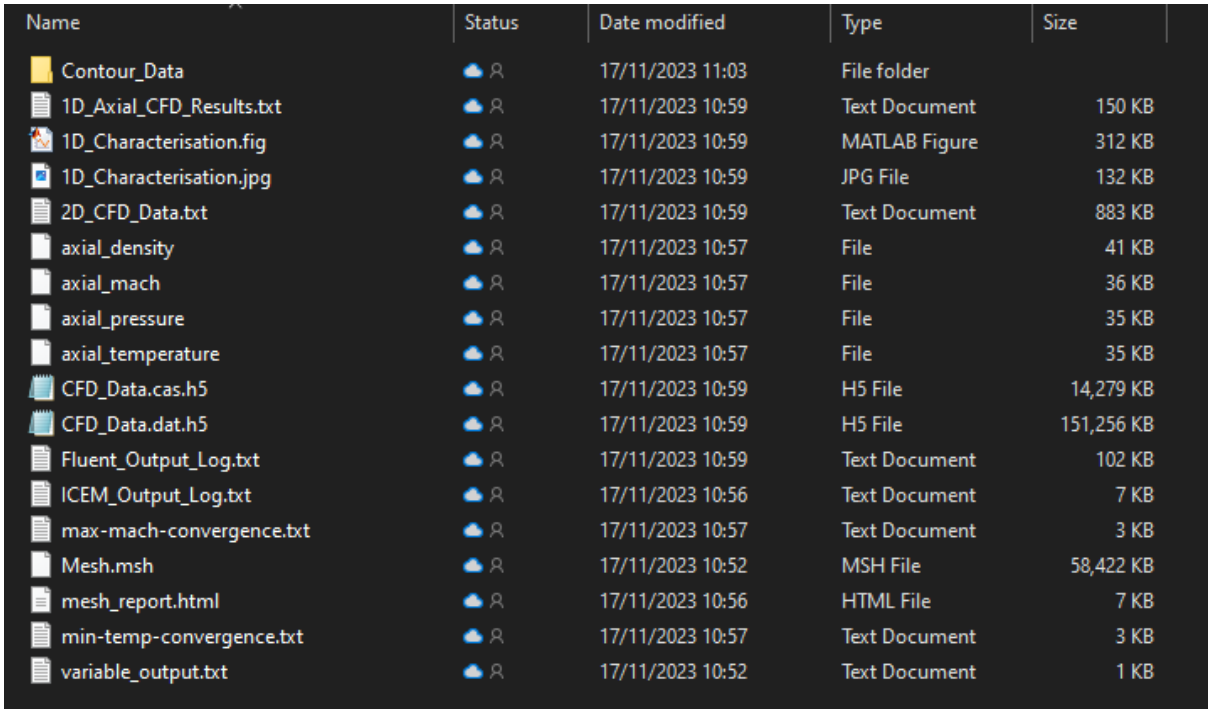
The main command required to run the study is.

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.

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 following files:



Name	Status	Date modified	Type	Size
Contour_Data		17/11/2023 11:03	File folder	
1D_Axial_CFD_Results.txt		17/11/2023 10:59	Text Document	150 KB
1D_Characterisation.fig		17/11/2023 10:59	MATLAB Figure	312 KB
1D_Characterisation.jpg		17/11/2023 10:59	JPG File	132 KB
2D_CFD_Data.txt		17/11/2023 10:59	Text Document	883 KB
axial_density		17/11/2023 10:57	File	41 KB
axial_mach		17/11/2023 10:57	File	36 KB
axial_pressure		17/11/2023 10:57	File	35 KB
axial_temperature		17/11/2023 10:57	File	35 KB
CFD_Data.cas.h5		17/11/2023 10:59	H5 File	14,279 KB
CFD_Data.dat.h5		17/11/2023 10:59	H5 File	151,256 KB
Fluent_Output_Log.txt		17/11/2023 10:59	Text Document	102 KB
ICEM_Output_Log.txt		17/11/2023 10:56	Text Document	7 KB
max-mach-convergence.txt		17/11/2023 10:57	Text Document	3 KB
Mesh.msh		17/11/2023 10:52	MSH File	58,422 KB
mesh_report.html		17/11/2023 10:56	HTML File	7 KB
min-temp-convergence.txt		17/11/2023 10:57	Text Document	3 KB
variable_output.txt		17/11/2023 10:52	Text Document	1 KB

The files names and information of these are summarised in the table below.

File/Folder Name	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.fig	MATLAB figure showing the 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, axial_mach, axial_pressure, axial_temperature	These files contain the raw data for each of the quantities across the flow axis (y = 0). These are not formatted and x = 0 relates to location of the nozzle inlet. Therefore, negative values will be in the reservoir. The 1D_Axial_CFD_Results are shifted by the nozzle length.
CFD_Data.cas.h5	This is the fluent case file that was setup by the code
CFD_Data.dat.h5	This it 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-mach-convergence.txt	This contains the maximum Mach 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.
Min-temp-convergence.txt	This contains the 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.
Variable_output.txt	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.

If you have any questions feels free to email me at scldr@leeds.ac.uk

Good Luck!