



N2 — Applied



SUSTAINABLE MANURE

DELIVERABLE

Modeling of the ScanArc thermal plasma torch

This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 965546

Deliverable number: 1.1

Due Date: 31-01-2022

Nature¹: R

Dissemination Level²:

Work Package: 1

Author(s): Colin O'Modhrain

¹Nature:

R = Report, P = Prototype, D = Demonstrator, O = Other, E = Ethics

²Dissemination level:

PU = Public

PP = Restricted to other programme participants (including the Commission Services)

RE = Restricted to a group specified by the consortium (including the Commission Services)

CO = Confidential, only for members of the consortium (including the Commission Services)

Restraint UE = Classified with the classification level "Restraint UE" according to Commission Decision 2001/844 and amendments

Confidential UE = Classified with the mention of the classification level "Confidential UE" according to Commission Decision 2001/844 and amendments

Secret UE = Classified with the mention of the classification level "Secret UE" according to Commission Decision 2001/844 and amendments

1. Introduction

The process of modelling is an incredibly useful tool for the design and optimisation of reactors and their operating systems. A key advantage to modelling compared to building and testing reactors is the reduction of production costs and time. A model can illuminate the potentially effective prototypes from a list of concepts in this way. In the instance of reactor improvements, well-built models can provide invaluable input during the redesign and optimisation, guiding the production team towards the end-goal of an efficient reactor. The latter is the aim for this model, as the three-dimensional model built using COMSOL Multiphysics software will provide insights into both the current operation of the ScanArc thermal plasma torch and potential improvements to the overall design.

2. Model overview

The modelling of the ScanArc thermal plasma reactor was approached in several consecutive stages, each of which was carried out using COMSOL Multiphysics (v5.6) software:

1. Build ScanArc reactor geometry
 - Built preliminary linearly scalable simplified reactor geometry (3D).
 - Optimised geometry for simulations.
 - Meshed reactor body and gas inlets.
2. Model gas flow component
 - Tested and compared different Reynold's Averaged Navier Stokes (RANS) turbulence models using steady-state solutions.
 - Examined the influence between incompressible (constant density) and compressible (density varying with temperature and pressure) flow.
 - Obtained steady-state and transient solutions for initial gas flow profiles (no plasma volume/heating effects present).
 - Refined the mesh *via* systematic study of relevant variables.
 - Elected to use laminar flow model as a simplifying assumption to the model.
3. Model heat transfer component
 - Added heat balance equation into the model, coupling this to the Navier-Stokes equations for gas flow with the common variable of density.
 - Obtained steady-state and transient solutions with this coupling to ensure model stability.
 - Added an artificial heat source diagonally across the reactor.
4. Model electrical component
 - Added current conservation equation.
 - Coupled electrical module with heat balance equation

- With the fully-coupled model (flow/heat/electrics) and the artificially enhanced ignition channel, produced a thermal arc within the simplified geometry.
5. Model simple chemistry
- Added simplified reaction set relevant to thermal air plasmas.
 - Used the solutions to fully-coupled model as input parameters (*e.g.* temperature and flow profiles)
 - Obtained and compared steady-state solutions for a range of flow rates and input powers.

3. Results

When building the ScanArc reactor geometry, a simplified version was chosen to ensure that the physics being modelled were accurate and self-consistent prior to application on the actual reactor geometry.

This reactor setup was then linearly scaled down by a factor of 50 to reduce the size of the computational domain and thus the computational time required to reach a solution

In terms of further reactor optimisation for the reduction of computational complexity, sharp edges and angles were rounded to reduce the incidence of non-converging solutions to the equations being solved in these areas. An example of this optimisation can be observed at the inlet-to-reactor connection (Fig. 1).

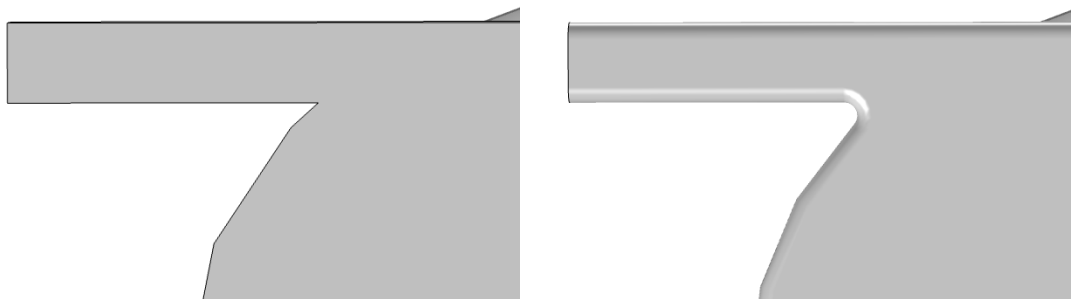


Fig. 1 Sharp angles before (left) and after (right) optimisation

The process of meshing a geometry is pivotal for the accurate resolution of problems when using the Finite Element Method (FEM) (*i.e.* the method employed by COMSOL Multiphysics software). In our case, this involves dividing the whole reactor into smaller sections (finite elements) within which the relevant equations will be solved. Naturally, the results obtained can vary depending on the quality of the mesh. A good quality mesh will provide an adequate number of elements in regions with large gradients in the problem solutions, allowing for these regions to be accurately captured. As a result, it is important to carry out regular mesh refinements by systematically observing variables of interest in these areas and ensuring the values do not vary dramatically

when altering the number of elements. Once these values no longer vary due to the number of elements describing a region, a point known as mesh convergence is reached. Each problem and new set of conditions should reach this point before any significant conclusions can be drawn.

To describe the flow fields within the reactor, the Navier-Stokes equations must be solved. Direct and stable solutions to these equations are very difficult to obtain using current computing resources. As a result, several different approaches have been developed to overcome these limitations, the least time-consuming of which is the process of Reynolds-averaging the equations (RANS modelling). The RANS models are time-averaged versions of the Navier-Stokes equations, and are used to describe turbulent flows. The RANS models investigated in the ScanArc geometry were the k-epsilon (k-ε), realizable k-epsilon (k-ε) and Menter’s Shear Stress (SST) models. These three models were compared with a simple laminar flow test case (*i.e.* no turbulent effects). In the ScanArc reactor, there is a significant swirling flow due to the combination of tangential inlets and high input gas velocities. Unfortunately, most of these models are not suitable for high-velocity, high-swirl flows, which was evidenced when the parameter of angular velocity (Eqn. 1) was examined (Fig. 2).

$$\text{Angular velocity [m/s]} = \frac{(x \cdot v - y \cdot u)}{\sqrt{x^2 + y^2}}$$

Eqn 1. Angular velocity
(v = y component of velocity) (u = x component of velocity)

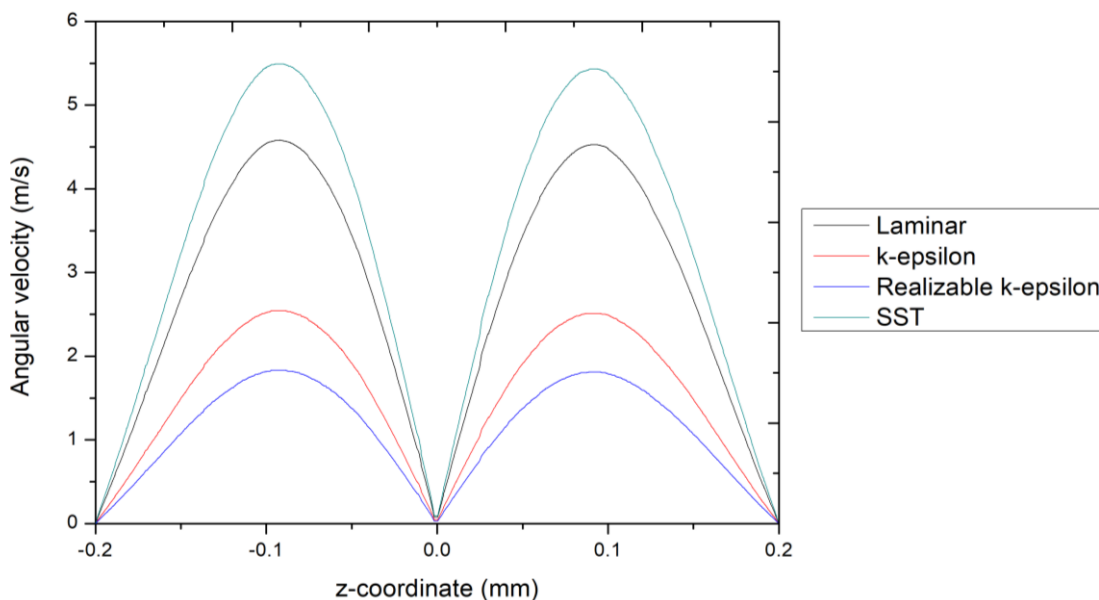


Fig. 2 Comparison of different flow models for angular velocity in simplified reactor(measured halfway along reactor)

The SST model appears to be the most adequate at resolving this complex problem. This is to be expected, as the SST model is a hybrid of the k- ϵ and k- ω models. The first is relatively accurate in the free stream while the latter shows good resolution in the near-wall region. The downside to the SST model is that the computational time is drastically higher than any of the other models, and the ability to reach a convergent solution is also significantly lower. However, examination reveals that the laminar flow model can also be used as an adequate assumption to solve this difficult flow problem. While some accuracy is lost by choosing this model, the amount of computational time saved and decrease in non-linearity of the problem are deemed a worthwhile trade-off.

Upon comparison of incompressible and compressible flow, it becomes evident that the latter is most certainly required for the modelling of plasma systems. The gradients in temperature and pressure resulting from arcs affect the gas flow profiles significantly. To capture these physical effects, it is clear that compressible flow (*i.e.* density dependent on both temperature and pressure) is required to capture all of the physical effects.

An investigation of the temperature within the reactor with varying applied current and constant flow rate was conducted. The higher current flowing through the arc results in more electromagnetic heating.

A comparison of the temperature profiles with velocity and pressure profiles from the same fully-coupled study was conducted. From a pressure plot, we can see that the gas expansion due to heating raises the pressure within the simulated reactor significantly, which further contributes to the high gas velocity near the outlet

4. Conclusion

A 3D thermal model of the ScanArc plasma torch was completed in COMSOL, allowing for insights into the underlying mechanisms and processes taking place.