CFD Modelling of the Temperature Profile in a Plasma-arc Furnace Reactor Quench Probe

Tobie D. Loftus, Joani van Rooyen, Abraham F. van der Merwe and Izak J. van der Walt

Abstract— Plasma gasification is the thermal decomposition process which utilises extreme temperatures to eliminate waste materials and produce a syngas product. The purpose of the quench probe is to withdraw the excess energy from a mixture of unstable gaseous species and is an extremely important step in determining the composition of the syngas product. The South African Nuclear Energy Corporation (Necsa) is currently developing a laboratory scale plasma-arc furnace reactor of which the quench probe operation and performance is yet to be evaluated and optimised. This study focusses on modelling the temperature profile in the quench probe using Computational Fluid Dynamics (CFD) simulations. This study investigates the effect of the following variables: (i) the product gas flow rate (ii) the current supplied to the plasma-arc torch and (iii) the flow rate of the quenching water. During the experimental phase five temperature measurements were taken along the length of the quench probe, which were further used to validate the developed CFD model. The number of parcel streams used in the CFD model was investigated and the selection of 20 parcel streams resulted in the most accurate model, with a root-mean square value of 7.38 °C. The developed CFD model accurately predicted the temperature profile in the quench probe, with an average error of 7.00 %. The velocity profile obtained from the CFD model indicated the existence of a stagnant gas flow zone, which causes heat transfer to propagate towards the gas inlet. Both the modelled and experimental results indicate that only the first spray nozzle in the quench probe is used for gas cooling at the investigated low temperatures, while the latter nozzles serve no purpose. The temperatures measured by the second thermocouple deviated from the modelled results on a number of occasions and the operation of this measuring device should be further investigated.

Index Terms—CFD modelling, Plasma gasification, Quench Probe

I. INTRODUCTION

Globally the amount of waste materials per capita is steadily rising while the human population also continues to grow at a rapid rate [1]. This leads to an increased demand for waste removal which is becoming increasingly unmanageable. This, along with the general public’s ever increasing environmental awareness, provides a drive-force to implement a sustainable and environmentally friendly waste removal strategy. Plasma gasification provides a unique solution to the waste removal problem.

Plasma gasification is an environmentally friendly process that has received a lot of attention in recent times due to its ability to eliminate waste materials as well as producing a syngas product [2]. The aim of this process is to convert the organic fraction of the waste materials into a syngas mixture, while retaining the inorganic fraction as an inert slag. The syngas product can be used as a fuel source, while the inert slag can be either advantageously reused or disposed of in a landfill.

Plasma gasification utilises the energy released by a plasma flame in order to extensively decompose the organic materials in the waste feed [3]. The organic decomposition takes place at extremely high temperatures; typical electrically generated thermal plasmas produce temperatures in the order of 2000 °C and higher [3].

The effluent gasses will have an extremely high temperature, due the excessive amount of energy absorbed in the reactor. The excess energy, in the product gas stream, is removed in the reactor quench probe, which is designed to reduce the gas temperature by means of injected water sprays. Water-cooled quenching systems are the most commonly used, although chemical quenching remains another alternative [4], [5]. The quench probe is specifically designed to rapidly decrease the gas temperature with typical cooling rates exceeding 10⁶ °C/s [6], [7].

The purpose of the quenching step is to cool the hot gaseous product in order to prevent the formation of complex species, thus promoting the hydrogen and carbon monoxide yield [2]. Plasma gasification systems ensure a steep temperature gradient, thus allowing the gas species to attain a non-equilibrium composition and preventing the formation of environmentally harmful substances, such as larger hydrocarbons, dioxins and furans. The main function of the quenching step is thus to control the product gas composition [4].

Previous studies indicate that higher quenching rates result in higher syngas yields which explains the need for the refinement and optimisation of the quenching step. Modelling the temperature profile within the quench probe will provide useful information which can be used to identify improvement areas in the design and operation of the probe.

Necsa have designed and implemented a laboratory scale plasma-arc furnace reactor, which is still in the development phase. Currently the syngas product contains relatively large amounts of carbon dioxide, indicating that the quenching step needs further improvement. Modelling the temperature profile in the quench probe will provide useful data for further optimisation studies.

The primary objectives of this study include: (i) developing a CFD model that describes the temperature profile in Necsa’s laboratory scale plasma-arc furnace reactor quench probe and (ii) validating the CFD model results by means of experimental measurements. Making suggestions in order to improve the quench probe operation is included as a secondary objective in this study.

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II. METHODOLOGY

A. Process description

A simplified schematic of the laboratory scale plasma-arc furnace reactor used for this study is displayed in Fig. 1.

Fig. 1. Simplified schematic of the plasma gasification process.

Argon is used as the start-up gas, while nitrogen is used after successful initiation to maintain a continuous plasma flame. A spark-plug is used with the purpose of providing the initiating energy needed in order to produce the plasma flame. After start-up, the nitrogen gas is fed to the plasma reactor torch at a specific flow rate in order to successfully maintain the plasma flame. An additional gas inlet can be found on the reactor, with the purpose of adding an additional air, oxygen or water feed to the reactor if required. A temperature of approximately 1000 °C is reached near the plasma jet, within the reactor, as a result of the heat transferred from the single DC non-transferred plasma torch. The hot gas generated in the plasma reactor passes through the quench probe where the temperature is rapidly decreased. The quench probe utilises five water spaying nozzles to cool the hot gas. The cooled gas/water mixture then exits the quench probe and passes through a filter system.

B. Experimental procedure

During the experimental phase of this study the effect of the following variables were investigated: (i) the gas flow through the quench probe (ii) the current supply to the plasma-arc torch and (iii) the flow rate of the quenching water. Table I summarises the experimental variations used in this study.

<table>
<thead>
<tr>
<th>Current Variations</th>
<th>Quench Water Variations</th>
<th>Gas Flow Variations</th>
</tr>
</thead>
<tbody>
<tr>
<td>130 A</td>
<td>All spray nozzles open</td>
<td>32.4 L/min N₂</td>
</tr>
<tr>
<td>140 A</td>
<td>First spray nozzle closed</td>
<td>32.4 L/min N₂ &amp; 65.0 L/min Air</td>
</tr>
<tr>
<td>150 A</td>
<td>First and second spray nozzle closed</td>
<td></td>
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</table>

Experimental temperature measurements were taken at five different points in the quench probe, WIKA® type K thermocouples were used to obtain these measurements. The temperature in the reactor was also continuously measured using a WIKA® type R thermocouple, due to the extremely high temperatures present in the reactor. The supplied water temperature was constantly monitored. Temperatures were logged with a Picolog® TC-08 USB thermocouple data logger.

The nitrogen and air flow rates were continuously measured using flow meters. Before the experimental runs proceeded, the gas flow meters were calibrated with a Gilibrator-2 flow calibrator. The water spray nozzles were each equipped with a valve and a calibrated liquid flow meter. The water flow rates were manipulated by adjusting the valve position and the flow rates were monitored and noted throughout all experimental runs.

The current supplied to the plasma reactor was varied by adjusting the power supply settings. The power supply is equipped with a current indicator and this value was noted regularly throughout the experimental runs. The pressure of the water supplied to the spray nozzles was monitored, in order to determine the spray nozzle characteristics.

Fig. 2 displays a representation of the quench probe geometry while Fig. 3 indicates the five different thermocouple locations.

Fig. 2. Representation of the quench probe geometry.

Fig. 3. Quench probe geometry and thermocouple positioning.

III. MODEL DEVELOPMENT

A. Assumptions

In order to simplify, whilst still ensuring model accuracy, the following assumptions have been made in the CFD model platform:

1. Water droplets injected by the spray nozzle were considered spherical particles.
2. Gas flow was considered turbulent.
3. Gasses were considered incompressible.
4. The gas entering the quench probe was considered to have a fully developed flow profile.
5. Heat transfer from all mechanical flanges was neglected.
6. Three-dimensional mass and heat transfer was considered.

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7. Only steady-state operation was considered.
8. Droplet evaporation was neglected, due to the low inlet gas temperature, mass flow and velocity relative to the quenching water.

After an extensive CFD results analysis, it has been found that the above mentioned assumptions do not have a large influence on the heat transfer in the quench probe and will be regarded as valid for the purposes of this study.

B. CFD model development

CFD modelling is an extremely useful simulation technique which is becoming increasingly popular when modelling complex fluid flow and heat transfer problems. This technique is characterised by the discretisation of the governing flow and heat transfer equations, such as the conservation of mass, energy and momentum relations, into the three-dimensional space of the given geometry [8]. After reference models and boundary conditions have been specified, the simulation program performs a set of iterations and converges to a solution. This technique was selected to model the temperature profile in the given quench probe. The Star-CCM+ CFD® simulation package was used for this purpose.

Fig. 4. Geometric representation of the CFD model developed for the plasma-arc furnace reactor quench probe.

Fig. 4 displays the geometry used for modelling purposes, which was constructed in Solidworks® and imported into Star-CCM®. On the geometry three regions have been defined, namely, the quench probe wall (grey), a velocity inlet (red) and a pressure outlet (blue).

In order to generate a three-dimensional mesh the polyhedral mesher, surface remesher and prism layer mesher CFD models were selected. A base size of 0.01 m, a minimum size of 0.0025 m and a target size of 0.005 m were selected for the meshing reference values.

All boundary conditions were obtained from the experimental measurements. Nozzles operate as solid cone injectors and were modelled in the same way. The droplet velocities, outer cone angles and droplet sizes were acquired from the nozzle manufacturer, where these nozzles have been extensively tested. The volume flow rate through each nozzle and the particle temperature was carefully noted during the course of the experiments.

The Lagrangian Multiphase CFD model was used to describe the multiphase flow. In order to ensure that mass and heat can be transferred between the continuous and Lagrangian phases the two-way coupling model was included. Turbulence effects were introduced in the CFD model by using the k-ε turbulence model. The system was considered as non-reacting due to the inert nature of the gas in the probe, while the segregated flow model was also implemented due to the incompressibility of the gas. The characteristics and models used in the CFD simulation are listed in Table II.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Modelling Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Meshing</td>
<td>Polyhedral and prism layer with surface remesher</td>
</tr>
<tr>
<td>Spray nozzles</td>
<td>Solid cone injectors</td>
</tr>
<tr>
<td>Droplet size</td>
<td>Constant particle size</td>
</tr>
<tr>
<td>Droplet-wall interaction</td>
<td>Escape model</td>
</tr>
<tr>
<td>Modelling approach</td>
<td>Lagrangian multiphase</td>
</tr>
<tr>
<td>Phase interaction</td>
<td>Two-way coupling</td>
</tr>
<tr>
<td>Turbulence model</td>
<td>k-ε turbulence model</td>
</tr>
<tr>
<td>Continuous phase</td>
<td>Incompressible, non-reacting gas with segregated flow</td>
</tr>
</tbody>
</table>

Another greatly important modelling specification for the nozzles is the number of parcel streams injected by each spray nozzle [9]. In the CFD modelling framework particles are not injected individually, but rather as groups of particles or parcels [10]. The number of parcel streams specifies the number of injected droplet streams and should be optimised in order to accurately represent the spray nozzle. Based on the model specifications, the Star-CCM® user guide suggests that the number of parcel streams should be between 10 and 100. In order to ensure accurate spray nozzle modelling this parameter will be investigated and adequately selected.

IV. RESULTS AND DISCUSSION

A. Parcel stream comparison

The developed CFD model was used to model all of the validated experimental temperatures, based on a variation in the number of parcel streams at each injector. This was done in order to find an optimal number of parcel streams to accurately model the temperature profile in the quench probe. Based on the guideline that the number of parcel streams for a solid cone injector should be equal to or larger than 10, the modelled results were investigated for 10, 20 and 30 parcel streams.

Fig. 5 clearly indicated the accuracy of each parcel stream variation by comparing the linearity of the relationship between the modelled results and experimental measurements. The results for 10 parcel streams (a) indicates a poor linear relationship and most of the data points can be found above the ideal prediction line, indicating inaccurate or skewed results. For 20 parcel streams (b) a strong linear relationship exists and most of the data points are scattered close to the ideal prediction line, indicating that the modelled results compare well with the experimental measurements. The third variation of 30 parcel streams (c) clearly shows a very strong linear relationship, although the data points are mostly located below the ideal prediction line which indicates inaccurate modelling.
The number of parcel streams used in the CFD model was further compared statistically in Table III, based on how well a linear regression line fitted the data points (R^2 value) as well as how much the modelled temperatures deviated from the experimental measurements which are given by the root-mean-square error (RMSE). The results clearly indicate that the model containing injectors with 20 parcel streams best describes the experimental data. This model has the lowest RMSE and a good linear fit. In Fig. 5(b) it can be seen that the linear regression line was only negatively affected by a poor fit for the three high temperature data points.

For further modelling purposes all injectors were assigned 20 parcel streams, as this selection best describes the experimental data.

### A. Model results

The developed CFD model displayed a consistent gas velocity profile and three comparable temperature profiles, depending on the number of spray nozzles operated.

![Fig. 6. Typical modelled temperature profiles for (a) all spray nozzles open (b) first spray nozzle closed and (c) first and second spray nozzles closed.](image)

<table>
<thead>
<tr>
<th>Model</th>
<th>R^2</th>
<th>RMSE (°C)</th>
</tr>
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<tbody>
<tr>
<td>10 Parcel streams</td>
<td>0.7297</td>
<td>11.83</td>
</tr>
<tr>
<td>20 Parcel streams</td>
<td>0.9265</td>
<td>7.379</td>
</tr>
<tr>
<td>30 Parcel streams</td>
<td>0.9612</td>
<td>10.23</td>
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TABLE III

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Fig. 7 displays the typical modelled velocity profile of the gas in the quench probe and clearly indicates that the current geometry causes the formation of a stagnant zone in the flow profile. This zone is characterised by recirculating gas flow, which results in gradual cooling near the gas inlet. This effect is clearly visible for the case where the first two spray nozzles are out of operation, depicted in Fig. 6 (c), while still being applicable when only the first spray nozzle is closed. Based on the CFD graphical outputs it can be noted that the recirculating flow pattern results in poor heat transfer characteristics in the stagnant zone, especially when the first spray nozzle is out of operation.

A. Model validation

Fig. 5(b) indicates the accuracy of the CFD model by comparing all modelled temperatures with the respective experimental measurements. However, this section focusses on validating the model accuracy for each of the experimental variation. Variations in gas flow through the probe, current supplied to the reactor as well as the quench water flow is considered. It is important to note that the experimental error was determined as 3.15 % and is thus not visible in the resulting graphs.

a) Pure nitrogen

This section contains the results for the case where the gas flow through the quench probe consisted of pure nitrogen, with a flow rate of 32.4 L/min.

The modelled temperature profiles for cases (a) and (c) correspond extremely well to the experimental measurements, for all of the different currents supplied to the reactor. Fig. 8(b) also shows a corresponding trend in the temperature profile, although a clear outliner can be seen. This can be attributed to a number of different factors. From the number of parcel streams comparison it can be seen that this parameter severely influences the model accuracy and can be further optimised in order to obtain improved results.

Furthermore, due to the recirculating flow region the temperature profile near the position of the second thermocouple varies significantly, especially when one or more of the quench probe spray nozzles are out of operation. If the thermocouple measuring location varies from the designed location, the experimental temperature will deviate from the modelled temperature. The temperature measurements were taken with the aim of measuring the temperature in the centre of the quench probe cross-section. The position of the second thermocouple can be further evaluated, in order to ensure accurate temperature measurements.

Both modelled and experimental results indicate that almost all of the gas cooling takes place at the first spray nozzle in operation. The succeeding spray nozzles serve no purpose as they provide no additional cooling.

b) Air/nitrogen mixture

This section contains the results for the case where the gas flow through the quench probe consisted of a 67.5 % air and 32.5 % nitrogen mixture, with a flow rate of 97.4 L/min.

The modelled temperature profiles fit the experimental data extremely well in cases (a) and (b), regardless of the current supplied to the reactor. For the case where the first two spray nozzles were closed (c) some deviations occurred. The most likely reason for this is model inaccuracies, such as the selection of the number of parcel streams. The modelling accuracy can be further improved by investigating a large range of variations in this parameter.

The outliner is once again present at the second thermocouple location, thus indicating that the position of this location
The experimental and modelled results indicate that only the first working spray nozzle influences the cooling rate in the quench probe. The use of five spray nozzles is excessive and unnecessary at the temperatures investigated in this study.

Both the modelled and experimental results indicate that only the first spray nozzle in operation is used for gas cooling. At the temperatures investigated, the latter nozzles serve no purpose and can be eliminated from the quench probe design. The modelled velocity profile clearly shows the formation of a stagnant zone, resulting in recirculating gas flow in this region. This allows the gas cooling to proceed gradually near the entrance, when the first nozzle is out of operation. This is undesirable and can be eliminated by adjusting the quench probe design or permanently utilising the first spray nozzle during quenching operations.

Once the plasma gasification system is fully commissioned and operated with an organic feed, the temperature in the reactor and the quench probe will increase. At these increased temperatures the latter spray nozzles might serve a bigger purpose and should be further investigated. At higher operating temperatures and gas flows, the assumption regarding the droplet evaporation might not be valid and should be re-evaluated.

Larger current supplies to the plasma gasification reactor resulted in higher operating temperature, while not influencing the trend in the temperature profile. The trend in the temperature profile for both the pure nitrogen gas and the air/nitrogen gas mixture is comparable, although the addition of air lead to much higher operating temperatures.

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