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Modelling, Simulation and Design of an Integrated Radiant Syngas Cooler and Steam Methane Reformer for use with Coal Gasification.

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ABSTRACT:

In this work, a novel process intensification design is proposed to integrate the Radiant Syngas Cooler (RSC) utilised to cool the coal-derived synthesis gas in entrained-bed gasifiers and a Steam Methane Reformer (SMR). The feasibility of the proposed integrated system is analyzed by developing a rigorous, dynamic, multi-dimensional model and establishing design heuristics for the integrated system. Two different flow configurations are explored; co-current and counter-current. The simulation results show that the proposed concept is feasible that allows for methane conversions as high as 80% in co-current mode and 88% in counter-current mode. The results also demonstrate that the counter-current design, though with higher conversion and cooling duty provided when compared to co-current designs, is limited by the tube wall material limitations. Our analysis shows that the total avoided CO₂ emissions is 13.3 tonnes/h by using the proposed integrated configuration in place of an external reformer for the natural gas feed rates considered in this study. In addition, a sensitivity analysis is performed on key model assumptions and the resulting effect on the performance is assessed. The sensitivity results have helped identify key factors to consider prior to pilot-scale implementation and further improvement for agile designs; a one third reduction in tube length reduced pressure drop by as much as 50% but reduces methane conversion by 15% points, neglecting slag deposition on tubes over-predicts performance only by 3%, and a 10% change in gas emissivity calculations affects model prediction of performance by less than 1%.
1. Introduction

Synthesis gas (commonly referred to as “syngas”) is a gaseous mixture where the major constituents are hydrogen and carbon monoxide. It is a key feedstock in the production of hydrogen, electricity, methanol, ammonia, synthetic fuels by the Fischer-Tropsch (FT) process, and commodity chemicals such as di-methyl ether (DME). Gasification and reforming are the two primary industrial routes available to produce syngas. The gasification path employs high temperature partial oxidation of solid fossil fuels like coal, biomass or carbon intensive waste products like petcoke and municipal solid waste. For reforming, a variety of hydrocarbons can be used as feedstock, but methane is the preferred feedstock in many of the hydrogen production facilities in the world [1]. Steam reforming of methane is an endothermic catalytic process where the heat required is supplied by combustion of fuel (usually natural gas) to the reactant gases (steam and methane) within multiple tubes that are placed inside a furnace. Though the product from both gasification and reforming is syngas, the quality of syngas varies widely between them. Moreover, each of these processes has unique advantages and disadvantages which are exploited depending upon the industry they are applied in.

One of the main advantages of gasification technology is that it allows for the consumption of vast available resources of solid fossil fuel reserves to produce fuels, chemicals and electricity, thereby reducing the reliance on oil, especially for nations that import crude oil but have large reserves of coal. The major disadvantage in using gasification for fuels and chemicals synthesis is the low $\text{H}_2/\text{CO}$ molar ratio in the product synthesis gas. The $\text{H}_2/\text{CO}$ molar ratio usually ranges from 0.75-1.1 depending upon the type of feed (coal/biomass) [2], which generally needs to be upgraded to a higher $\text{H}_2/\text{CO}$ ratio depending on the application (for example, Fischer-Tropsch (FT) synthesis requires a feed ratio of 2 [2] but some DME synthesis routes require a feed ratio of 1.2-1.5 [3]). The gas is usually upgraded by
employing Water Gas Shift (WGS) reactor that converts carbon monoxide and steam to hydrogen and carbon dioxide. This process, however, leads to a loss in the plant-wide carbon efficiency (ratio of total carbon atoms in products to total carbon atoms in the input to the plant), increased carbon dioxide emissions and higher capital and processing costs. Alternatively, reforming is an established technology especially in petroleum refineries, and the resulting syngas is hydrogen rich with a molar H\textsubscript{2}/CO ratio of greater than 3. However, the disadvantage is that the Steam Methane Reforming (SMR) process is highly endothermic necessitating combustion of natural gas to supply the heat required resulting in CO\textsubscript{2} emissions. Clearly, there is an opportunity to improve performance of syngas production processes using synergistic options with reduced emissions. Bhat and Sadhukhan [4] present an excellent review on the possibilities for improving SMR technology using different process intensification strategies, one of which involves using heat integration with exothermic or high temperature systems to supply heat to the endothermic reactions. Considering the need to find more efficient plants that incorporate sustainable designs, the advantages of each of these independent technologies can be harnessed by integrating them together in one unit that will result in efficiency improvements, flexible capability to meet different H\textsubscript{2}/CO molar ratios for downstream processes and reduced emissions.

One such application was studied by Adams and Barton [2] who explored integrating natural gas steam reforming with coal based entrained-bed gasifiers as shown in Figure 1. The integrated design resulted in an increase in the total system efficiency (compared to non-integrated equivalent processes) by up to 2 percentage points and an increase in net present value of up to $100 million for a polygeneration plant of 1711 MW (equivalent to 227 TPH of coal feed). The concept was centred on the need to cool the high temperature coal-derived synthesis gas exiting the gasifier at 1600 K to 1020 K (conventionally done using steam generation in a radiant cooler with tubes) and the steam methane reforming process requiring heat to drive the endothermic reactions. The heat integration strategy involves placing tubes in the radiant cooler filled with SMR catalyst. The proposed integrated configuration resolves the issue
of meeting the desired H\textsubscript{2}/CO ratio without WGS reactors or external reformers. The proposed configuration also envisioned dynamic operational capability. It is attractive because there are significant potential economic advantages if the products of downstream processes can be changed periodically to respond to market demands and prices [5]. Currently, this is difficult to do in part because the gasifier which forms the upstream part of the plant exhibits poor dynamic operability. However, by integrating gasification and steam methane reforming into one unit, it is possible to change syngas production quality and rate dynamically while keeping the gasifier itself at steady state.

Though Adams and Barton [2] showed that this integrated system was attractive from a systems-level techno-economic perspective, the feasibility of such a device itself was never studied in any level of detail. The authors acknowledged the need to develop and study the integrated device in order to determine key design parameters, product yields and qualities, conversion efficiencies, costs, controllability, dynamic operating envelopes, and other performance criteria. Therefore, the primary focus in this work is to develop first-principle based multi-scale, dynamic, heterogeneous model to address these issues and propose an initial base-case design. To the best of our knowledge, this is the first work to propose a specific design for the integrated concept, develop a corresponding model, and study its performance in detail.

2. Materials and Methods

The development of the multi-scale, dynamic, heterogeneous model for the integrated system is explained in this section. The model consists of five sub-models that are coupled to simulate the hybrid system. The five sub-models include the (1) refractory lining of the RSC, (2) coal-derived syngas inside the RSC, (3) tube wall of the SMR tubes, (4) gas phase inside the tubes and (5) catalyst particles that are packed within the tubes. Both co-current and counter-current configurations for the tube gas flow have been analyzed and presented. It should be noted that the gasifier, that precedes the RSC, has not been
modelled in this work as the key idea behind the proposed configuration is to operate the gasifier at steady-state and not to subject it to the dynamic transients of a polygeneration plant.

2.1 RSC Shell Model

The RSC Shell model includes mass balances, energy balances, and a pseudo momentum balance for the shell syngas phase. The model accounts for the spatial and temporal variations in concentration and temperature of the shell gas phase. The following principal assumptions have been made:

1. The pressure drop in the radiant cooler is small (on the order of 1 bar [6]) and therefore does not need to be modeled using rigorous first principle equations. Instead, the pressure drop has been fixed and assumed to be linear with respect to vessel length.

2. The shell side coal-derived syngas is assumed to contain particles of very small diameter of less than 10 µm (ash and other impurities from gasification) that get entrained with the gas, as suggested by Brooker [5]. The effect of the particles on the total gas emissivity has been considered (See supplementary material).

3. The coal-derived syngas inside the RSC is well mixed and no radial variations in concentration and temperature are considered. As such, each SMR tube is assumed to be identical, a common assumption applied to a similar arrangement of tubes in SMR furnaces [8], [9].

4. Molten slag has not been considered in this work. In entrained bed gasifiers, the liquid slag from gasification flows along the gasifier walls and at the RSC inlet, it drops to the bottom as droplets into the quench pool [7][10]. The residence time for the molten slag droplets in the RSC is small enough compared to the gas such that the heat transfer from the slag to the walls is considered negligible.

5. Slag deposition on tube surfaces was considered and found to have a relatively small impact on the final design (see Section 6.3). Since neglecting slag deposition increases the speed of simulation, it was not considered for most of the results in this work.
2.1.1 Shell Gas Phase Mass Balance

The dynamic component mass balance in the shell is given by:

\[
\frac{\partial c_{i,s}}{\partial t} = - \frac{\partial (c_{i,s}v_s)}{\partial z} + r_i, \quad (1)
\]

where \(c_{i,s}\) is the concentration of species \(i\) in the shell gas stream, \(v_s\) is the downward velocity of the gas and \(r_i\) is the rate of WGS reaction of component \(i\). The boundary condition at \(z=0\) is \(C_{i,\text{inlet}}\).

On the shell side, the coal-derived synthesis gas consists of \(\text{H}_2\), \(\text{CO}\), \(\text{CO}_2\), and \(\text{H}_2\text{O}\) and hence exothermic WGS reactions occur and need to be accounted for in the RSC model. Though Monaghan and Ghoniem [11] mention that the WGS reactions in the radiant cooler do not have a major effect on the exit coal-derived syngas composition, there is a need to include WGS kinetics to predict the RSC exit temperature with better accuracy. There are numerous WGS kinetic models available for catalyst based systems that operate below 450°C [12] but few are available for homogenous reaction systems such as for gasification chambers. However, the homogenous kinetics for WGS in a combustion environment is used in this work and is given as follows [13], [14]:

\[
r_i = 2.75 \times 10^9 \exp\left(-\frac{10100}{T_{g,s}}\right)\left(C_{\text{CO}}C_{\text{H}_2\text{O}} - \frac{1}{K_{\text{eq}}} C_{\text{CO}_2}C_{\text{H}_2}\right) \quad (2)
\]

where \(T_{g,s}\) is the shell gas temperature, \(C_{\text{CO}}\) is the concentration of carbon monoxide, \(C_{\text{H}_2\text{O}}\) is the concentration of water vapour, \(C_{\text{CO}_2}\) is the concentration of carbon dioxide, \(C_{\text{H}_2}\) is the concentration of hydrogen and \(K_{\text{eq}}\) is the equilibrium constant. Note that in the above equation, the concentration and pre-exponential factor are in the units of kmol/m\(^3\) and m\(^3\)/kmol.s respectively that will have to be changed to the required units of mol/m\(^3\).s for the \(r_i\) term. The equilibrium constant is given by the following equation [14]:

\[
K_{\text{eq}} = \exp\left[470.8524 - 175.8711(\ln T_{g,s}) + 21.95011(\ln T_{g,s})^2 - 0.9192934(\ln T_{g,s})^3\right] \quad (3)
\]
2.1.2 Shell Gas Phase Energy Balance

The model considers radiative and convective heat transfer between coal-derived synthesis gas on the shell side and tube walls and also between the coal-derived synthesis gas and the refractory lining. It should be noted that the reflection from the refractory lining to the tube wall was considered negligible. However, the effect of this assumption on model prediction is studied in section 6.3. The dynamic gas phase energy balance is given by the following equation:

\[
\frac{\partial (\rho_{\text{molar,s}} H_s)}{\partial t} = -\frac{\partial (\rho_{\text{molar,s}} H_s)}{\partial z} - \frac{N_t}{A_s} (Q_{t,\text{rad}} + Q_{t,\text{conv}}) - \frac{1}{A_s} (Q_{r,\text{rad}} + Q_{r,\text{conv}}),
\]

where \(H_s\) is the enthalpy of the gas phase in the shell, \(N_t\) is the number of tubes inside the RSC, \(\rho_{\text{molar,s}}\) is the gas molar density, \(A_s\) is the cross-sectional area of the shell, \(Q_{t,\text{rad}}\) and \(Q_{t,\text{rad}}\) is the heat transferred by radiation from the gas stream to a single tube wall and the refractory lining respectively, \(Q_{t,\text{conv}}\) and \(Q_{r,\text{conv}}\) is the heat transferred by convection from the gas stream to a single tube wall and the refractory lining respectively.

The enthalpy of the gas phase is defined as follows:

\[H_s = \sum_{i=1}^{N_c} H_i y_i,\]

where \(H_i\) is the enthalpy and \(y_i\) is the mole fraction of component \(i\) in the gas phase. The enthalpy of the component \(i\) is given by the following equation:

\[H_i = \Delta H_{\text{form},i} + \int_{T_{298}}^{T_g,s} C_{p,i} dT,\]

where \(\Delta H_{\text{form},i}\) is the heat of formation and \(C_{p,i}\) is the temperature dependent specific heat capacity of component \(i\) in the gas phase.

The heat transfer terms by radiation and convection between the shell gas and tube wall are computed as:

\[Q_{t,\text{rad}} = \sigma \varepsilon_g \varepsilon_t \left( \pi D_{t,o} \right) \left( T_{g,s}^4 - T_w|_{r=R_{t,o}}^4 \right),\]

\[Q_{t,\text{conv}} = h_{g,s} \left( \pi D_{t,o} \right) \left( T_{g,s} - T_w|_{r=R_{t,o}} \right)\]
\[ Q_{r,rad} = \sigma \epsilon_g \epsilon_r \left( \pi D_{s,i} \right) \left( T_{g,s}^4 - T_r^4 \bigg|_{r=R_{s,i}} \right) \] (9)

\[ Q_{r,conv} = h_r \left( \pi D_{s,i} \right) \left( T_{g,s} - T_r \bigg|_{r=R_{s,i}} \right) \] (10)

where \( \epsilon_r \) is the emissivity of the refractory, \( D_{s,i} \) is the inner RSC shell diameter, \( T_{r(=R_{s,i})} \) is the inner refractory temperature and \( h_r \) is the convective heat transfer coefficient between the gas phase and the refractory lining. The boundary condition at the inlet \( z=0 \) is \( T_{s,inlet} \).

2.2 SMR model

The heterogeneous model used in this work for catalytic steam methane reforming is from our previous work [15]. The SMR model accounts for the spatial and temporal variations in the gas and catalyst particle. For model and auxiliary equations, reaction kinetics and more details the reader is advised to refer to the prior work and fundamental model equations are provided in the supplementary material.

2.3 Tube Wall Model

The model for the SMR tube wall accounts for the transient heat conduction along the axial and radial direction. In our previous work [15], a similar two-dimensional model was presented assuming a planar tube wall. The model has been changed where the thin slab wall approximation has been removed to account for the radial curvature of the wall for improved accuracy and is as follows:

\[ \rho_t C_p \frac{\partial T_w}{\partial t} = \lambda_t \left[ \frac{\partial^2 T_w}{\partial r^2} + \frac{\partial^2 T_w}{\partial z^2} \right], \] (11)

where \( T_w \) is the tube wall temperature, \( \rho_t \) is the density \( (7880 \text{ kg/m}^3) \), \( C_p \) is the specific heat capacity \( (741 \text{ J/Kg-K}) \) and \( \lambda_t \) is specific thermal conductivity \( (28.5 \text{ w/mK}) \) of the tube material[16].
2.3.1 Tube Wall Boundary Conditions

The outer wall of the SMR tube is subjected to radiative and convective heat flux from the shell side gas as described in section 2.1.2. The boundary condition at \( r = R_{t,o}, \forall z \) and \( t > 0 \) is given as:

\[
\lambda_t \left[ \frac{\partial T_w}{\partial r} \right]_{r=R_{t,o}} = \sigma \varepsilon_t \varepsilon_t (T_{g,S}^4 - T_w^4)_{r=R_{t,o}} + h_{g,s} (T_{g,S} - T_w)_{r=R_{t,o}}.
\]

(12)

The tube emissivity \( \varepsilon_t \) is 0.85 [17].

At the inner wall, the heat transfer to the process gas or the tube side gas is by convection. The boundary condition at \( r = R_{t,i}, \forall z \) and \( t > 0 \) is given as [15]:

\[
\lambda_t \left[ \frac{\partial T_w}{\partial r} \right]_{r=R_{t,i}} = h_w(T_w)_{r=R_{t,i}} - T_{g,t}.
\]

(13)

At the top and bottom of the tube wall, flux is assumed to be zero because of the small cross sectional area [15]. The boundary condition at \( z = 0 \) and \( z = L, \forall r \) and \( t > 0 \) is given as:

\[
\left[ \frac{\partial T_w}{\partial z} \right]_{z=0} = \left[ \frac{\partial T_w}{\partial z} \right]_{z=L} = 0.
\]

(14)

2.4 Refractory Model

The proposed integrated system design does not arrange the tubes into a tightly-packed “waterwall” configuration along the inside of the refractory as is often done in a conventional RSC for a GE gasifier, where high pressure steam is generated. Instead, the SMR tubes are arranged in a circle inside the shell near the edge, but with some spacing between the shell and the tubes, as well as between the tubes themselves (see Section 4). However, the RSC shell needs to be protected from the high temperature environment and hence the proposed design envisages the use of a refractory lining. Also, refractory lining provides insulation as in conventional coal-fired furnaces and reduces the heat dissipation to the surroundings. In an entrained-bed gasifier, the refractory is typically composed of different layers typically consisting of fireclay brick, insulating brick and a castable layer [6] [11]. However, because detailed refractory layout is outside the scope of this work, only a single layer of firebrick refractory is modelled with “average” properties. The model is similar to the tube wall model and is given as:
\[ \rho_r C_{p_r} \frac{\partial T_r}{\partial t} = \lambda_r \left[ \frac{\partial^2 T_r}{\partial r^2} + \frac{\partial^2 T_r}{\partial z^2} \right], \]  

(15)

where \( T_r \) is the refractory temperature, \( \rho_r \) is the density (2645 Kg/m\(^3\)), \( C_{p_r} \) is the specific heat capacity (960 J/Kg-K) and \( \lambda_r \) is specific thermal conductivity (1.8 w/m-K) of the refractory material [18]. It should be noted that, if desired, additional layers can be added to the model without great difficulty.

2.4.1 Refractory Boundary Conditions

At \( r = R_{RSC,l} \), \( \forall z \) and \( t > 0 \), the inner wall of the refractory is subjected to convective and radiative heat flux from the shell gas.

\[ -\lambda_r \frac{\partial T_r}{\partial r} \bigg|_{R_{RSC,l}} = \sigma \varepsilon_r \varepsilon_r \left( T_{g,s}^4 - T_r^4 \bigg|_{R_{RSC,l}} \right) + h_{g,r} \left( T_{g,s} - T_r \bigg|_{R_{RSC,l}} \right), \]  

(16)

where \( \varepsilon_r \) is the refractory emissivity and \( h_{g,r} \) is the convective heat transfer coefficient from the shell gas to the refractory inner wall. The \( \varepsilon_r \) is commonly assigned a constant value of 0.83 [10], but it should be noted that the emissivity changes significantly with temperature. The emissivity values provided in the supplementary material for the refractory were fit to a second order polynomial model as a function of temperature and then used in the simulations given as follows:

\[ \varepsilon_r = -1 \times 10^{-7} T_r^2 + 8 \times 10^{-5} T_r + 0.8935 \]  

(17)

At the outer wall of the refractory, heat is exchanged with ambient air via radiation and convection. The boundary condition at \( r = R_{RSC,o} \), \( \forall z \) and \( t > 0 \) is given as:

\[ -\lambda_r \frac{\partial T_r}{\partial r} \bigg|_{R_{RSC,o}} = \sigma \varepsilon_r \varepsilon_r \left( T_r^4 \bigg|_{r=R_{RSC,o}} - T_{amb}^4 \right) + h_r \left( T_r \bigg|_{r=R_{RSC,o}} - T_{amb} \right) \]  

(18)

At the top and bottom of the refractory lining, the flux is assumed to be zero because of the small cross sectional area [15]. The boundary condition at \( z = 0 \) and \( z = L, \forall r \) and \( t > 0 \) is given as:

\[ \frac{\partial T_r}{\partial z} \bigg|_{z=0} = \frac{\partial T_r}{\partial z} \bigg|_{z=L} = 0 \]  

(19)

3. Model Validation for Independent Systems

The model presented in this work is for a proposed integrated configuration and no experimental data exists to validate the model predictions for the integrated device. The key motivation towards the
development of a model has been to evaluate the feasibility of the proposed integrated configuration
and develop a base case design that can help cut costs when building the pilot-scale system. Though a
certain percentage of design margin will be included to account for the model mismatch with the real
system, it is essential to show that the model predictions are within a certain confidence interval where
the results can be considered reliable to analyze the performance of the integrated system. To this end,
the approach that was adopted in this work for model validation was to validate the models for the SMR
and RSC independently. Considering the limitations, this is the best methodology possible to validate
the integrated model.

The SMR model was validated in the prior work with four industrial data sets available in the open
literature. The model showed great accuracy with a maximum deviation of 5.38 % points between the
model prediction and data for methane conversion [15]. The RSC shell model validation, in comparison,
is more challenging because in the conventional GE gasifiers, the radiant cooler cools the hot coal-
derived syngas by generating high pressure steam in a waterwall configuration. Robinson and Luyben [6]
simulated the radiant cooler in Aspen using CSTRs in series with a constant coolant temperature of 608
K assuming the RSC consisting 2828 tubes with a diameter of 2 in. They also mention that very few
references are available about the design. Kasule et al. [19] followed a similar approach to simulate the
RSC, where a PFR was used with a constant coolant temperature of 609 K. Monaghan and Ghoniem [11]
also employ a PFR configuration to simulate the radiant cooling, where they note that saturated vapour
at the exit of the waterwall is at a temperature and pressure of 608.9 K and 137.8 bar respectively [20].
Furthermore, design and material details for the radiant coolers are sparse and contradictory. For
example, references [6], [21], state that the RSC diameter is 16 feet (4.877 m) and length is 100 feet
(30.48 m). In another available reference [20], the authors mentioned that the assumed RSC diameter
(inner) is 2.74 m with a length of 40 m. Also, details about material properties like the thermal
conductivity, density or specific heat capacity are not available. The data sets that were used for model validation, with certain material properties assumed, are tabulated in Table 1.

The method employed in this work to validate the RSC Shell model assumes a ring of tubes along the circumference of the RSC to mimic the waterwall, where steam is generated within the tubes. The temperature of the tube inner wall is assumed to be at the steam temperature of 609 K instead of the boundary condition described in Eq. 13. The number of tubes in the waterwall that can fit along the circumference of the gasifier is calculated by dividing the circumference of the gasifier by the outer diameter of the tube. For data set 1, using this approach, the number of tubes is 282 while it is 122 for data set 2. The model prediction for exit mole fractions of the gaseous components using data set 1 is shown in Figure 2. It can be seen from the predicted mole fraction of the gaseous components that the rate of WGS reaction is higher when compared to the reported simulated data. This increased rate is because the WGS rate equations were developed for hydrocarbon combustion where the reactions proceed at a much faster rate. This fact is also acknowledged by Monaghan and Ghoniem [11] when using the same reaction kinetics model and instead they used the rate equations by Bustamante et al. [22], [23] for simulating the WGS reactions in the RSC. However, Monaghan and Ghoniem still had to tune the predicted rates to around “0-8%” of that predicted by Bustamante’s expression to match the available data sets. The same strategy could well have been adopted in the current work but were not done for two reasons; (i) the range of 0-8% varies depending on the data set employed and (ii) the rate equations developed by Bustamante et al. [22], [23] were for temperatures in the range of 1070 K-1134 K (for forward WGS reaction) and 1148 K to 1198 K (for reverse WGS reaction), well below the operating temperature of the RSC where the inlet temperature is greater than 1600 K and the exit temperature is in the range 866 K to 1089 K. The model prediction for the RSC exit temperature is 914 K compared to the reported simulated exit temperature of 866 K [6]. However, for the same data set, the design temperature reported for the Tampa power plant, where the RSC is employed, is 1033 K while the
operating temperature is below 1005 K [24]. This shows that with the limited available data and with no parameter estimation, the model prediction for RSC exit temperature falls within an acceptable range of around 5% between the two reported temperatures. For data set 2, the model prediction for the exit mole fraction is shown in Figure 2 and compared against the reported model prediction and equilibrium composition reported by Monaghan and Ghoniem [20]. It can be seen that the mole fraction prediction differs marginally from the reported simulated data but matches with the equilibrium composition reported. However, it was noted that increasing the length changed the molar composition which implies that equilibrium has not been attained. The temperature at the RSC exit is predicted to be 975 K compared to the reported temperature 1089 K [20]. Though the relative percentage error is around 10.5%, it should be accounted that the model has not been modified accurately to represent an actual membrane wall configuration. Also, other effects like slag deposition (considered by the authors) on the wall have been ignored that offer resistance to heat transfer across the walls. This is the principal reason for the predicted drop in temperature compared to the model used by Monaghan and Ghoniem [20] where slag phase temperature was tracked.

Therefore, it is reasonable to conclude, with all the afore-mentioned limitations and considering the fact that the objective is to analyze the design and operability of a new hybrid system for which experimental data is non-existent, the model prediction for the individual systems i.e. the SMR and RSC is sufficient to explore the proposed hybrid configuration.

4. Determination of Design Parameters for the Hybrid System

To simulate the integrated system, several design parameters are required as inputs to the model. The key design parameters are the RSC shell diameter, RSC shell length, refractory thickness, tube length, tube diameter and number of tubes within the RSC shell. It is evident that there are several design parameters and a good starting point to determine the values is using a retro-fit approach. Using this technique, the proposed integrated system is first designed for existing entrained-bed gasifiers in the
industry. For the tube side design parameters, conventional SMR tube diameters include tubes with outer and inner diameter of 0.1-0.084, 0.102-0.0795, 0.114-0.102, 0.115-0.1 and 0.1322-0.1016 m respectively [25]–[30]. However, the number of tubes inside the RSC is influenced by two contrasting characteristics; (i) the physical space limitation within the RSC shell and (ii) required surface area based on the cooling duty to be provided.

To determine the number of tubes that can fit inside a given RSC shell diameter, the placement of the tubes inside the RSC was treated as a typical fired-heater where the tubes are placed in an annular arrangement in 2 rows along the refractory lined wall. In Figure 3, “C” represents the centre to centre distance between the tubes and “D” represents the outer diameter of the tube. The number of tubes that can be placed depends on the C/D ratio. The C/D ratio can either be 1.5 or 2, but the ratio adopted in this work is 2, as this ensures uniform flux around the circumference of the tubes [31]. The distance between the refractory lined wall and the tube centre is 1.5 times ‘D’. Based on the adopted design properties, the total number of tubes for a single row within the RSC shell is given as:

$$N_t = \frac{\pi(D_{RSC}-2D_{lo})}{(\frac{3}{2})D_{t, o}}$$

Equation 20 gives the upper limit to the number of tubes that can be fit in a single row as a function of the RSC shell diameter, tube diameter and C/D ratio. However, the question remains if the available surface area is sufficient to provide the required cooling duty for a commercially operating gasifier with a coal-feed rate of 102 tonne per hour that requires 2.54 GJ/tonne coal [2] which equals to 72 MW. Conventional SMR tubes are known to operate with an average heat flux of 45 kW/m$^2$ to 90 kW/m$^2$ while modern high flux reformers operate at 116 kW/m$^2$ [32]. The average flux through the tube walls for the integrated system has been used as a gauge to determine the operation severity [33]. Therefore, the base-case design should be able to provide the minimum cooling duty of 72 MW and the average heat flux should fall between the above-mentioned ranges. Of the tube diameters considered, a smaller tube diameter with a small wall thickness was chosen (0.1 m-0.084 m) to fit more tubes and also to
reduce the weight as the total weight is directly proportional to the diameter [34]. Using equation 20, the number of tubes were 137 assuming two rows of tubes along the refractory wall. However, results are also presented to demonstrate the availability of multiple designs with different tube lengths and diameters.

5. Numerical Analysis and Grid Independence Test

The model consisting of partial differential and algebraic equations was implemented in gRPOMS v3.7.1, an equation-oriented process modeling environment [35]. The method of finite differences was utilised to discretize the spatial domain that includes the axial direction along the length of the RSC, the radial direction within the catalyst particles and the lateral direction for the tube wall and refractory lining. A centred finite difference scheme was used for the radial domain of the catalyst particles (4\textsuperscript{th} order) and for the lateral domain of the tube wall and refractory (2\textsuperscript{nd} order). For the axial domain, backward/forward finite difference scheme was used depending upon the flow configuration.

The grid size determines the accuracy of the model solution but the trade-off of using a fine grid is the computation time associated with a large model as described in this work. Considering the fact that the future applications of the proposed model were to analyze dynamic performance and control design, the effect of grid fineness on computation time was important, and ensuring the accuracy of the model prediction simultaneously. In numerical methods, accuracy is generally determined by comparing computed value against a true value or the relative percentage change from the previous iteration meets a set tolerance. One way to determine if a grid size is appropriate is to track the percentage change in one of the variables until it meets a specified tolerance. More often than not, one of the key properties that are neglected in the simulation of first-principle models is the global conservation of mass and energy. With huge models, especially those that incorporate several coupled sub-models, a simple but effective way to analyze the accuracy of a particular grid and model validity is to check if the fundamental mass and energy balances are conserved.
In this work, the model was simulated using different grid sizes for the axial and radial domains, keeping the lateral domain for the walls constant at 10 nodes. It was observed that mass within the tubes and the shell was always conserved for different mesh fineness (axial domain) where the relative difference between the inlet and outlet was of the order $10^{-7}$. However, the mesh fineness affected the energy conservation significantly because unlike mass which was not flowing between the tube side axial domain and the shell side axial domain, energy was flowing across these domains. Therefore, the conservation of energy between the shell and tube side was evaluated using the following equation:

$$\Delta E = E_{shell} - (E_{tube} + E_{ref})$$

(21)

where $E_{shell}$ is the energy change between the inlet and outlet shell side streams, $E_{tube}$ is the energy change between the inlet and outlet tube side streams and $E_{ref}$ is the energy transferred to the refractory wall from the shell side gas. The cumulative function is then calculated on a normalised basis for both $\Delta E$ and CPU time, which is given as follows:

$$CF = \left( \frac{\Delta E}{\Delta E_{max}} \right) + \left( \frac{CPU ~ time}{CPU ~ time_{max}} \right)$$

(22)

As the grid gets finer, the energy balance difference will tend towards zero but at the expense of a huge CPU time. The cumulative function, described in equation 22, combines the effect of conservation and CPU time which is plotted as a function of axial and radial nodes as shown in Figure 4. From Figure 4, it is evident that the optimal grid size lies at 75 axial nodes, 35 radial nodes with a cumulative function value of 0.6157. However, it is interesting to note that increasing the radial nodes to 50 has a minimal impact on the cumulative function, while the axial nodes have maximum impact. Therefore, a fine grid with 75 axial nodes and 50 radial nodes was adopted in this work for greater accuracy. With this grid size, energy balance is closed to around 1% and the CPU time required is 11 minutes.

6. Results and Discussion

6.1 Performance of Co-current and Counter-current Configurations
The dynamic model developed was initialised using a warm start-up case. The warm start-up state was obtained by introducing a nitrogen feed at a temperature of 727.4 K in the tube side and by using an equimolar feed of carbon dioxide and water (products of combustion from gasifier burners used during gasifier start-up) at a temperature of 727.4 K. Once steady-state was attained, feed with conditions given in Table 2 was introduced on the tube and shell side. The simulation continued until steady-state and the results were then used to analyze the performance.

Figure 5 shows the steady-state temperature and conversion profiles along the axial length in both co-current and counter-current configurations. The coal-derived syngas on the shell side is cooled to a temperature of 1123 K and 977 K in the co-current and counter-current configuration respectively. This results in a cooling duty provided of 73.5 MW for the co-current configuration and 91 MW for the counter-current configuration. On the tube side, for co-current flow, the process gas exits at a temperature of 1063 K while for the counter-current flow configuration the exit temperature is 1179 K. The coal-derived syngas exit temperature in commercially operating RSC’s that employ steam generation to provide the required cooling ranges from 866 K to 1089 K as described in section 3. Comparing the RSC shell exit temperatures of the proposed integrated design, the co-current configuration falls slightly outside this range while the counter-current flow falls well within the specified operating range in commercial plants. However, the improvement with the proposed design is the high value product on the tube side. It can be seen from Figure 5 that methane conversion on the tube side is sufficiently high at 80% for co-current configuration and a very high 88% for counter-current configuration. In literature, the reported methane conversion for industrial SMR reactors ranges between 65% to 90%. On the shell side, as the temperature of the coal-derived syngas decreases along the axial length, the exothermic WGS reaction is favoured as shown in Figure 5. In both configurations, CO conversion is around 20%. These results demonstrate two key performance objectives that the proposed design had to meet: (i) provide the required cooling duty and cool the hot coal-derived syngas
and, (ii) show that the available exergy is sufficient to integrate a highly endothermic SMR operation with high methane conversion. With the key performance objectives demonstrated, it is imperative to know if the proposed system is violating any operating constraints. The key operating constraints pertaining to this design include the following: (i) temperature at which refractory failure occurs, (ii) average flux through the SMR tube walls and (iii) maximum tube wall temperature. The refractory brick failure temperature is set at 2073 K [20] for the inner wall and 573 K for the outer wall. Figure 6 shows the axial temperature profiles for the refractory layer (both inner and outer wall) for both co-current and counter-current configuration. It can be observed that the temperature of the outer layer of refractory exceeds the safety limit for the initial 5 m and hence the refractory thickness will need to be increased. It was observed that a 25% increase in refractory thickness from the base case 0.2 m was sufficient to reduce the temperature to acceptable safety limits. Another option to circumvent this problem in the real system is to use either a thicker layer of refractory and/or a different refractory material along the axial length where temperatures exceed the specified limit; in this case for the initial 5 m. Figure 6 also shows the incident flux on the tube walls at every axial node along with the average flux for both the configurations. For co-current flow, the average flux through the tube walls is 45 kW/m² and for counter-current flow, the average flux is 56 kW/m². Even though the average flux through the tube walls lies within the range of commercially operating SMR plants, one of the key constraint violations to look for is the maximum tube wall temperature. The tube wall temperatures are a critical operating parameter that determine tube failures and by extension, the life of the tubes [34]. Available references from literature mention existing tube materials where reformers are designed for a maximum operating tube wall temperature of 1323 K [32], [36]. Also, commercial vendors have different tube materials available for petrochemical steam reformers which have a maximum temperature limit in the range 1273 K to 1448 K [37]. In this work, the maximum design limit temperature is set to 1350 K. Figure 6 shows the axial outer tube wall temperature profiles for both the
co-current and counter-current configurations. For the co-current flow configuration, the maximum tube wall temperature is 1181 K and for the counter-current configuration, the maximum tube wall temperature is close to the design limit at 1334 K. It should be noted here that the total flow rate through the tubes for the counter-current configuration was increased by 10% from 1061 kmol/hr (used for the co-current configuration) as the maximum tube wall temperature was 1375 K indicating the opportunity to process higher feed rates.

Another potential problem during nominal operation of the integrated system may be the incidence of a phenomenon termed as “metal dusting” that affects conventional steam reformer tubes. Metal dusting refers to the disintegration of the tube material into dust that includes fine metal particles and oxides. The typical temperature range at which metal dusting occurs in reformers has been established between 723 K and 1073 K. A study by Chun et al [38] on different Nickel based alloys showed that the maximum for localized metal dusting occurred at around 923 K. In our case studies, the tube wall temperatures (both inner and outer) lie outside this range at steady-state. However, the tube wall temperatures may lie in that range during start-up scenarios and while transitioning between different steady-states. It may well be possible that the more recent high performance tube materials (such as alloys resistant to metal dusting) can withstand the afore-mentioned constraints but the promising feature of this study has been to ensure operability with prevailing industry standards.

Both these base-case configurations are able to provide the minimum required cooling duty of 72 MW and high methane conversion. As mentioned previously, the co-current configuration processes 1061 kmol/hr of natural gas feed achieving a methane conversion of 80%. If the same conversion were to be attained using an external reformer assuming the same operating conditions, 264.6 GJ/hr of heat would be required that would be provided by combustion of natural gas. This would result in approximately 13.3 tonnes of CO₂ per hour if we consider 53.1 Kg of CO₂ is emitted per million Btu of energy supplied by natural gas combustion [39]. This shows that the proposed integrated system reduces the carbon
emissions when compared to using an external reformer. It should be noted that the numbers do not include the CO₂ avoided if the coal-derived syngas were to be upgraded using WGS reactors which would further increase the total avoided CO₂ when using the integrated system.

6.2 Other Design Options

Furthermore, the effect of different tube lengths and tube diameters from the base case designs was analyzed for the co-current configuration considering it was the more feasible design when compared to the counter-current configuration. For all of the cases considered, the feed conditions were set to the same as used for the base case design analysis. Table 3 shows a summary of the performance for each of the different cases considered. It was observed for the base case tube diameter that when the length was reduced to 20 m (approximately 33% reduction), the system was still able to provide a significant cooling duty of 67 MW to coal-derived syngas but the methane conversion dropped by 15 percentage points to 68%. However, the advantage with using shorter tubes is the significant reduction in pressure drop by around 50%. The low methane conversion can be improved by optimizing the operating parameters like the steam to carbon ratio in the feed, inlet temperature to the tubes or the inlet pressure. This allows space to explore for more agile designs that can improve upon the base case design performance. The analysis also shows the effect of different tube diameters and tube thickness on the performance; case 2 which has the thickest tubes has a significantly high maximum outer tube wall temperature. Additionally, larger outer tube diameters reduce the number of tubes that can be placed inside the shell which in turn increases the inlet feed rate per tube if the same amount of natural gas has to be processed. This in turn affects the inlet velocity and has a pronounced effect on the methane conversion. For example, case 2 with a length of 30 m provides almost the same cooling duty as the base case tube diameter with the same length but the methane conversion drops by 8 percentage points. This demonstrates the various degrees of freedom available such that the performance can be improved significantly using optimization techniques.
6.3. Sensitivity Analysis on Performance

It has been demonstrated in section 6.2 that the several designs are available for the proposed integrated configuration that meets all the key requirements of the process. However, it is important to acknowledge the fact that the designs are based on model predictions and identify how some parameters and assumptions will affect the performance of the proposed integrated configuration. The effect of (i) gas phase emissivity, (ii) radiation from refractory walls and (iii) slag deposition on tubes is considered in this section. For the sake of brevity, the following sections describe the results for co-current configuration while the results for the counter-current configuration can be obtained from the supplementary material.

The gas phase emissivity used by previous researchers, an important parameter for calculating the radiation heat transfer, range from 0.3 [40] to 0.9, while the maximum gas-particle total emissivity employed in similar modelling works is 0.9 [19], [41]. To assess the effect, the gas phase emissivity was then subjected to a +/-10% change. Five key parameters that demonstrate performance and operating constraints were chosen to evaluate the effect and percentage change from the base case value. In the following figures (Figures 7A-D), green bars indicate a favorable change and a red bar indicates a change that is not favorable for that parameter. For example, a decrease in the maximum tube wall temperature will be a favourable change which improves tube life while a decrease in the exit tube gas temperature is not a favourable change as this will lead to reduced methane conversion. For -10% change in the gas phase emissivity, Figure 7A shows that the effect on the performance is negligible with the methane conversion and cooling duty provided dropping by a mere 0.89% and 0.63% respectively. The maximum tube wall temperature drops by 1.7% which is favorable. For a +10% change, the opposite trend is observed as the heat transfer increases. The percentage change in methane conversion and cooling duty provided increase by 0.76% and 0.5% respectively while the maximum tube wall temperature increases by 1.5%. Though this change seems to be unfavourable, a 1.5% change translates
to a temperature of 1198 K, which is still within the design limit temperature and improves the performance.

Refractory materials are usually coated with a reflective coating that increases the capacity to re-radiate heat back to the furnace chamber minimizing heat loss to the environment. The assumption in this work of no heat transfer between refractory and tube wall might not be bad for evaluating the overall performance because if the heat loss to the environment is minimised it would only result in an increase in conversion of methane. However, the effect of that assumption might be critical for tube wall temperatures and was analysed by treating the shell as an adiabatic chamber. Figure 7C shows the effect on the designated parameters. As expected, methane conversion increases by 3% and 2% in co-current and counter-current configurations respectively. However, it is interesting to note that the cooling duty decreases. This is because in the base case simulations, the shell side gas exchanges heat with the refractory layer which in turn is cooled by the ambient air on the outside. This provides additional cooling to the coal-derived syngas. Also, the effect on the maximum tube wall temperatures was minimal as shown in Figure 7C. This shows that the effect of excluding complex radiation modeling has only a minimal effect on the model prediction.

The assumption of no slag deposition may hold true during initial stages of operation but an end of run analysis to determine performance depreciation due to slag buildup is beneficial. A slag layer of thickness 2 mm was considered on the tube surface, typically found in syngas radiant coolers in gasifiers. The model was modified to include an additional two-dimensional slag model on the tube surface. Figure 7D shows that the methane conversion and cooling duty provided decrease by 2.8% and 2.5% for co-current configuration. However, the slag buildup protects the tube walls from high temperature and the maximum tube wall temperature drops by 6.5%. This trend is especially significant for counter-current design where the base case maximum tube wall temperature was close to the design limit.
7. Future Work

With the base-case design and feasibility of the proposed integrated system established, future work will look at the dynamic operability of the proposed designs. It is critical to analyse the capacity of the proposed integrated system in transient modes of operation as the initial work by Adams and Barton [2] envisioned the application of such an integrated system to provide dynamic flexibility in a polygeneration plant. Also, an open loop analysis of the proposed system will help determine critical operating vulnerabilities. Another future work will focus on developing a robust control for the proposed integrated system. It should also be noted that the base case design presented here is sub-optimal where the performance can be maximised by optimising the operating parameters. Also, the assumption of homogenous tubes inside the RSC needs to be addressed using complex CFD models before pilot scale testing.

8. Conclusions

This work presented the design for a process intensification strategy for syngas production using gasification and methane reforming. A dynamic, multi-dimensional model was developed for the integrated system to study feasibility and performance. The results presented showed that the integrated configuration conceived by Adams and Barton [2] is a promising design option requiring further analysis before industrial implementation. The model predictions showed that the integrated design is capable to meet the required performance objectives that were set for a polygeneration plant. The co-current configuration was able to process a total natural gas feed rate of 1061 kmol/hr achieving a methane conversion of 80% without violating any of the set design constraints. In the process, the co-current design provided a cooling duty of 73.5 MW to the hot coal-derived syngas. However, for counter-current configuration, it was observed that the maximum tube wall temperature exceeded the design limit of 1350 K by 25 K for the same flow rate. A counter-current configuration with increased NG processing capacity of 1165 kmol/hr was demonstrated that met all the design constraints. The
simulations showed that both the flow configurations had different advantages and disadvantages. For example, the co-current configuration while providing a lower cooling duty when compared to counter-current design, the maximum tube wall temperature was far lower than that in counter-current flow. On the other hand, the counter-current flow configuration was able to achieve very high methane conversion but with higher tube wall temperatures. The results from the sensitivity analysis highlighted the aspects to be considered when pilot-scale implementations of the proposed system are done. The results also showed the advantages of shorter tubes with a significant reduction in the pressure drop but with a loss in performance because of a decrease in available heat transfer area. However, the results lay the foundation for exploring smaller and agile design configurations with lower NG capacity for new gasifiers that are not limited by retro-fit constraints. The authors acknowledge that the analysis of a new design based on models, even when rigorous, will be subjected to a certain degree of error due to the several assumptions and parameter uncertainties. However, such modelling efforts lay the groundwork for proof of concept that help support further research exploration into new and innovative reactor designs.

Acknowledgements:

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Nomenclature

Subscripts

\( c \) catalyst  
\( s \) shell  
\( conv \) convection  
\( t \) tube  
\( e \) effective  
\( r \) refractory  
\( g \) gas phase  
\( rad \) radiation  
\( i \) component indices  
\( w \) tube wall  
\( mix \) mixture

Variables

\( a_v \) \( \text{m}^2/\text{m}^3 \) catalyst external surface  
\( N_c \) - number of components  
\( C \) \( \text{mol/m}^3 \) concentration  
\( p \) bar partial pressure  
\( C_{p} \) \( \text{J/mol/K} \) specific heat capacity  
\( P \) bar total pressure
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
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<tr>
<td>D</td>
<td>m</td>
<td>diameter</td>
</tr>
<tr>
<td>( F_{\text{total}} )</td>
<td>mol/s</td>
<td>total molar flow rate</td>
</tr>
<tr>
<td>( G )</td>
<td>w/m²/K</td>
<td>mass velocity</td>
</tr>
<tr>
<td>( h )</td>
<td>w/m²/K</td>
<td>heat transfer coefficient</td>
</tr>
<tr>
<td>( H )</td>
<td>J/mol</td>
<td>enthalpy</td>
</tr>
<tr>
<td>( K_{\text{eq}} )</td>
<td>-</td>
<td>equilibrium constant</td>
</tr>
<tr>
<td>( L )</td>
<td>m</td>
<td>tube length</td>
</tr>
<tr>
<td>( \rho_{\text{molar}} )</td>
<td>mol/m³</td>
<td>density</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>w/m²/K⁴</td>
<td>Stefan-Boltzmann constant</td>
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<td>( \epsilon )</td>
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<td>emissivity</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>w/m/K</td>
<td>thermal conductivity</td>
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**REFERENCES**


Appendix:

A1. Gas Phase Correlations

The convective heat transfer coefficient from the shell gas to the tube wall is given by [41]:

\[ h_{g,s} = \frac{\lambda_{g,s}}{D_{o,t}} \left( 0.027N_{Re,t}^{0.8}N_{Pr}^{0.33} \right) \]  \hspace{1cm} (11)

where \( \lambda_{g,s} \) is the shell gas phase thermal conductivity, the Reynolds number \( N_{Re,t} = \frac{D_{o,t} \rho_s \mu_{g,s}}{\lambda_{g,s}} \) and the Prandtl number \( N_{Pr} = \frac{C_p \mu_{g,s}}{\lambda_{g,s}} \).

The convective heat transfer coefficient from the shell gas to the refractory wall is given by [18]:

\[ h_r = \frac{\lambda_{g,s} f(N_{Re,s} - 1000)N_{Pr}}{D_{s,l}\left(1 + 12.7\frac{L}{B}\right)^{0.5} N_{Pr}^{2/3}} \]  \hspace{1cm} (12)

where \( f \) is the friction factor and the Reynolds number \( N_{Re,s} = \frac{D_{s,l} \rho_s \mu_{g,s}}{\lambda_{g,s}} \).

The gas phase emissivity calculations are provided in the supplementary material and the value is 0.82.

Figure Captions:

1) Figure 1: Proposed concept of integrating RSC of an entrained-bed gasifier with SMR
2) Figure 2: RSC model validation using data sets 1 and 2
3) Figure 3: Placement of tubes within RSC shell

4) Figure 4: Determination of the optimal numerical grid size
5) Figure 5: Axial profiles of gas temperature and conversion in co-current and counter-current configuration
6) Figure 6: Axial profiles of refractory temperature, outer tube wall temperature and heat flux through tube wall for co-current and counter-current configuration
7) Figure 7: Sensitivity analysis for co-current configuration
Table 1: Available RSC Shell dimensions

<table>
<thead>
<tr>
<th>Design Parameter (m)</th>
<th>Length</th>
<th>Inner Diameter</th>
<th>Outer Diameter</th>
<th>Tube outer diameter</th>
<th>Tube thickness</th>
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<td>Data set 1 [6], [21]</td>
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<td>4.877</td>
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<td>Data set 2 [20]</td>
<td>40</td>
<td>2.74</td>
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<td>0.01</td>
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Table 2: Operating conditions for integrated RSC-SMR system

<table>
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<tr>
<th>Parameter</th>
<th>F_in,total (kmol/hr)</th>
<th>T_inlet (K)</th>
<th>P_inlet (bar)</th>
<th>Mole fraction</th>
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<td>CO: 0.2868</td>
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<td>N₂: 0.034</td>
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Table 3: Comparison of co-current system performance with different SMR tube thickness and length against base-case design

<table>
<thead>
<tr>
<th>Design</th>
<th>Base-case Tube diameter (0.1-0.084 m)</th>
<th>Tube diameter = 0.132-0.102 m</th>
<th>Tube diameter = 0.114-0.102 m</th>
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<tbody>
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<td>Case 1</td>
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<tr>
<td>Case 2</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td>L=30 m</td>
<td>L=20 m</td>
<td>L=30 m</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>--------</td>
<td>--------</td>
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<tr>
<td>Gasifier Capacity (TPH)</td>
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<tr>
<td>NG Feed Processed (kmol/hr)</td>
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<tr>
<td>Number of tubes</td>
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<td>102</td>
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<tr>
<td>Shell Gas Exit Temperature (K)</td>
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<td>Tube Gas Exit Temperature (K)</td>
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<tr>
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