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Development of an Entrained Flow Gasifier Model for Process Optimization Study

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Coal gasification is a versatile process to convert a solid fuel in syngas, which can be further converted and separated in hydrogen, which is a valuable and environmentally acceptable energy carrier. Different technologies (fixed beds, fluidized beds, entrained flow reactors) are used, operating under different conditions of temperature, pressure, and residence time. Process studies should be performed for defining the best plant configurations and operating conditions. Although “gasification models” can be found in the literature simulating equilibrium reactors, a more detailed approach is required for process analysis and optimization procedures. In this work, a gasifier model is developed by using AspenPlus as a tool to be implemented in a comprehensive process model for the production of hydrogen via coal gasification. It is developed as a multizonal model by interconnecting each step of gasification (preheating, devolatilization, combustion, gasification, quench) according to the reactor configuration, that is an entrained flow reactor. The model removes the hypothesis of equilibrium by introducing the kinetics of all steps and solves the heat balance by relating the gasification temperature to the operating conditions. The model allows to predict the syngas composition as well as quantify the heat recovery (for calculating the plant efficiency), “byproducts”, and residual char. Finally, in view of future works, the development of a “gasifier model” instead of a “gasification model” will allow different reactor configurations to be compared.

1. Introduction

Coal gasification is an attractive process to convert a solid fuel into syngas (which means synthesis gas, a mixture containing mainly hydrogen and CO), which can be further converted and separated to obtain hydrogen, a valuable and environmentally acceptable energy carrier. Although gasification is a relatively old process, the versatility of the process (with production of syngas, electricity, hydrogen, or chemicals) and the multiplicity of technological solutions (fixed beds, moving beds, fluidized beds, and entrained flow reactors) make it a current topic of investigation. A further motivation of renewed interest in this technology is the combination of gasification with advanced operations of gas clean up and separation, e.g. hot gas clean up for sulfur removal at high temperature and membranes for H₂ separation and CO₂ capture. These steps are fundamental to maximize the hydrogen production and purity. Also, heat recovery and management is a crucial issue to efficiently connect all units of these processes in integrated gasification combined cycles (IGCCs). In all cases, process studies should be performed for defining the best plant configurations and optimizing the operating conditions.^{1–4}

The core of a gasification plant is the gasifier, which can be realized under very different solutions.⁵ The heat needed can be provided by partial oxidation of coal with air or pure oxygen. Steam may be added to promote gasification. In some cases also recirculation gas streams (containing CO₂) may contribute to gasification. The coal can be fed dry or in a slurry. Temperatures, pressures, and residence times vary in wide ranges depending on the technological configuration. For

instance, fluidized beds work at moderate temperatures (800–1000 °C), while temperatures of 1500 °C can be even achieved in entrained flow reactors. Also solutions for heat transfer are various (jackets, heat exchangers, water, or gas quenches).

In spite of all these differences, most process studies in the literature modeled the gasifier as an equilibrium reactor.^{6–10} This approach is indeed fundamental for a preliminary study but hardly suitable for process analysis and optimization procedures. As a matter of fact, the reactors are developed to maximize the coal conversion, the hydrogen production (or the heating value of the syngas), and minimize tar formation. This is usually pursued through high temperatures or relatively long residence times. In these conditions, the assumption of equilibrium can be accepted, but only in terms of syngas composition. Some issues arise when introducing this hypothesis in optimization studies:

1. The gasification temperature is generally considered independent of other operating conditions; therefore, syngas compositions as functions of the oxygen-to-coal ratio can be found at fixed temperatures.^{6,7} This may be a useful exercise for equilibrium evaluations but hardly suitable for practical applications. In the real reactor, an increase of oxygen in the feed gives a higher temperature in the gasifier. Therefore, these two parameters can not be assumed independent of each other but should arise from a global heat balance, including reaction heat (devolatilization, combustion, and gasification) as well as feed heating. Also, heat recovery should be included, when steam or hot water production is realized. This contribution may be crucial for the global efficiency of the process but can be hardly derived from equilibrium assumptions.

2. The composition of the syngas can be arguable in some cases. CH₄ and CO₂ are generally underestimated even though their values are fundamental for process efficiency. Residual char is not predicted in equilibrium calculations, while the conditions for complete conversion should be determined to

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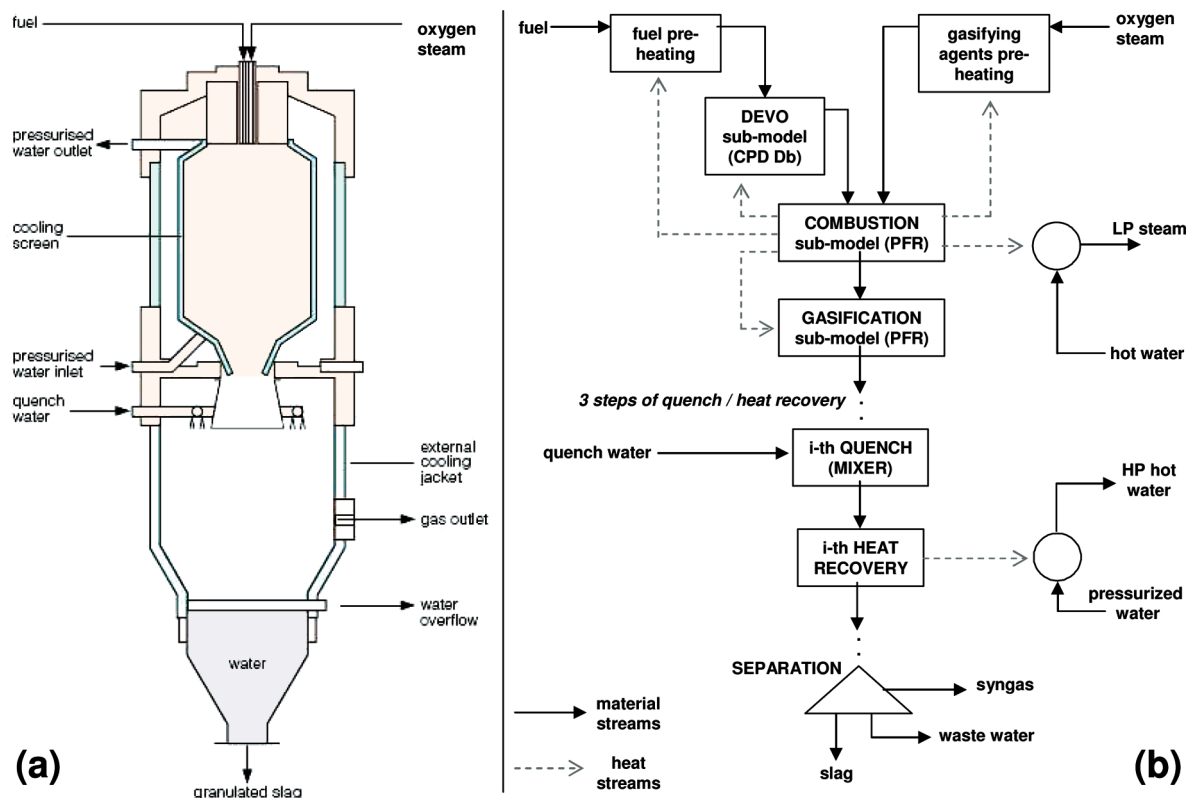


Figure 1. Scheme of the gasifier (a) and the model approach (b).

ensure high efficiencies and avoid problems in downstream units. Similarly, tar is not predicted in most studies: its quantification is actually fundamental to estimate the quality of the syngas produced and assess the necessity of including a tar-cracking section.

3. Gasification is a complex ensemble of chemical and physical phenomena. Each step can be studied under different conditions (of temperature and/or gaseous composition) and the optimal configuration of gasifiers (e.g., entrained flow reactors, fluidized beds, circulating beds, fixed beds) can be compared only by developing a detailed model. This is also the case of reactors which can be hardly represented with an equilibrium reactor (e.g., due to the low temperatures and residence times achieved).

For all the above points a “gasifier model” should be developed instead of a “gasification model”. So, the aim of this work is the development of a gasifier model to be inserted in a comprehensive process model for the production of hydrogen via coal gasification. The software used is AspenPlus. An entrained flow gasifier is modeled as a multizonal model by considering all chemical and physical steps from the reactant feeding to the cooling of the syngas produced. All steps are linked by material and heat streams according to the reactor configuration. Design parameters (e.g., residence time, heat transfer) are inserted in the model. The optimization of the operating conditions is the target of the work.

2. Reactor Description

The reactor studied is an entrained flow reactor with quench water (technology of Future Energy GmbH, recently acquired by Siemens,^{11,12} scheme in Figure 1a). The pressure generally is between 20 and 40 bar.⁵ The gasification reactions occur in the top section where pulverized dry coal is fed through a burner along with substoichiometric oxygen (from an air separation

unit). Very high peak temperatures are achieved, so steam can be added to promote endothermic gasification reactions between coal and water. Furthermore, a cooling screen shields this part of the gasifier and recovers heat for the production of low pressure steam. A cooling jacket for the production of pressurized hot water envelops the entire reactor. The high gasification temperatures give no tar in the syngas and melt the ash, thus forming a slag on the reactor walls. This slag is cooled and removed by the quench water in the bottom part of the gasifier. Granulated slag is removed from the bottom, while wastewater contains particulate ash matter, residual char and tar, and traces of soluble compounds (sulfur, nitrogen, heavy metals). The produced syngas leaves the reactor at a temperature of approximately 200 °C.

In this work the pressure is fixed at 30 bar and the effect of pressure variations is not studied. No hypothesis is made on the gasification temperature because it is derived from a heat balance, as discussed in the following section. A South African coal (moisture 7.0, volatile matter 24.8, fixed carbon 54.5, ash 13.7 wt % as received basis; C 81.6, H 4.84, N 1.75, S 1.27 wt % dry and ash free basis) is considered in all cases. The particle size is 0.1 mm. A flow rate of 5000 kg/h is assumed. This is a relatively small plant size, which may represent an attractive solution for a realistic starting scenario based on hydrogen economy. Pure nitrogen (99% vol) is used to feed the coal on a nitrogen-to-coal ratio of 0.05 wt/wt. A stream of pure oxygen (95% vol) is available from an air separation unit. Also, high pressure steam (31 bar) is available for gasification.

3. Gasifier Model Development

The gasifier model is entirely developed in AspenPlus in view to be linked to the other unit models of the hydrogen production process (e.g., gas cleanup, CO shift, H₂ separation). The gasification is divided into the main mechanisms acting in the

reactor. Each step is described by the representative equations adopting conventional blocks of AspenPlus or dedicated models opportunely implemented in the main code of the gasifier model. The separation is made considering the effective sequence of the physical/chemical mechanisms in the real gasifier and their characteristic time.

The gasifier model is then a multizonal model formed by submodels which are consecutive in the material streams, but interconnected in the heat streams as represented in Figure 1b. The main blocks are the following:

- fuel preheater
- gasifying agents preheater
- fuel devolatilization
- combustion
- gasification

- quench and heat recovery The models of each step are detailed in the following subsections.

3.1. Fuel and Gasifying Agents Preheater. The coal flow rate is initially treated as a nonconventional solid in AspenPlus and then divided into three streams according to the proximate analysis: water (considering the moisture content), ash, and the organic matter. Each stream is heated to the peak temperature (to be determined at this point), which coincides with the temperature of the following devolatilization step (described below), in a conventional heater block. Also gaseous streams (oxygen, steam, and nitrogen, for the transport of coal) are heated to the same temperature in heater blocks.

The heat to both blocks is provided by the combustion step, which also provides the heat for devolatilization and gasification steps and for the steam production. The scheme of the heat streams is shown in Figure 1b. The heat balance is implemented by connecting all these heat streams to a heat mixer block. The exit of this block gives the sum of all streams and represents the heat surplus (positive total) or the heat dispersion (negative total). The sign depends on the peak temperature, which coincides with the final temperature of preheating, devolatilization, and combustion temperatures as well as the initial temperature of gasification. This assumption is motivated when considering the high heating rate of the entrained flow reactors.¹ A design specification is imposed in the global model which varies the peak temperature to find the value corresponding to zero dispersion or heat surplus. The procedure is iterative (the peak temperature determines the extent of the reactions in all steps), so that the solution is obtained once all heat and mass balances are solved.

3.2. Devolatilization Submodel. The stream of the organic matter from the coal enters the devolatilization submodel. This step is assumed to be instantaneous thus interactions between solid and gas are not considered. The temperature coincides with the peak temperature. A thermal decomposition is modeled giving a solid residue (char), a condensable organic product (tar, here modeled as anthracene, $C_{14}H_{10}$), and the main gaseous species. In this work, the considered gaseous species are the following: CO, CO₂, CH₄, H₂O, H₂, C₂H₂, N₂, NH₃, HCN, H₂S, COS.

No conventional AspenPlus block can represent this step. Therefore, a structural model is considered, i.e. the CPD (coal percolation devolatilization, originally developed by Fletcher et al.¹³ in the form adapted by our group in previous works^{14,15}) for the coal devolatilization. This model gives the yield of macropducts and the speciation of gases once the coal composition and the operating conditions are known.

The Genetti correlation¹⁶ is used to obtain the CPD parameters from the ultimate and proximate analyses of the coal. As

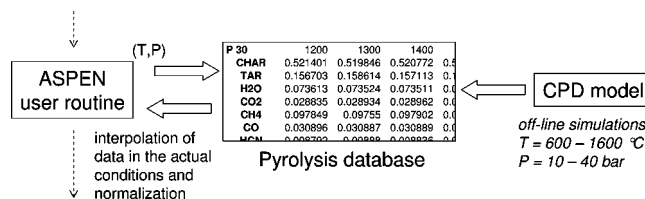


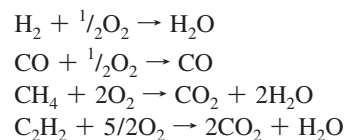
Figure 2. Scheme of the devolatilization block.

for the conditions, the CPD code can be hardly implemented in AspenPlus because of the expensive computational cost. Therefore, a user routine for the devolatilization step (scheme of Figure 2) is developed. Basically, it consists of a database and a calculation function. The former is created with the results of offline simulations of the CPD model in a wide range of pressures (10–40 bar) and temperatures (600–1600 °C), maintaining a high heating rate (10^4 °C/s) in all cases. The calculation function dialogues with the main AspenPlus model by receiving the actual values of temperature and pressure, interpolating the results of the database, and returning the balanced products. It is worth mentioning that the peak temperature is obtained iteratively to solve the design specification described above.

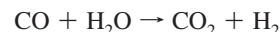
This procedure is efficient and accurate once a sufficiently crowded database is created. Temperature intervals of 100 °C are suitable in this case, while at temperatures higher than 1600 °C, the syngas composition does not vary to any further extent.

3.3. Combustion Submodel. The subsequent step is the combustion submodel represented as a plug-flow reactor, where combustion reactions consume oxygen:

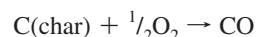
volatile combustion



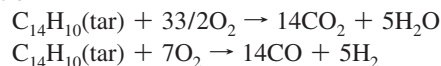
water–gas shift



char oxidation



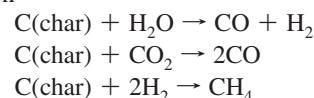
tar oxidation



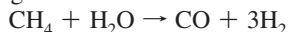
All of these reactions are modeled assuming a first order kinetic model with parameters adapted from literature works.^{15,17,18} The residence time is assumed to be 1/10 of the total residence time of the reactor (this latter is inserted according to the value suggested by the producers), and this assumption forces the oxygen to be consumed in all cases studied. The temperature is set constant at the peak value, obtained from the thermal balance described above.

3.4. Gasification Submodel. The gasification submodel consists of a plug-flow reactor. The reactions are the following:

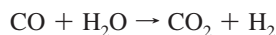
char gasification



methane reforming



water–gas shift



Homogeneous reactions are modeled assuming a first-order kinetic model with parameters from the literature.^{19–21} As for char gasification, the unreacted core-shrinking model was actually adapted from the work of Wen and Chaung.²⁰ In that work, the effective kinetics varied with the actual size of the solid particle, that is the ratio of the unreacted core radius and the entire particle radius. This approach is too complex to be implemented in the main AspenPlus model. So, constant values are assumed by averaging the kinetic parameters at the external surface and at the core of the particle. This approximation allows the kinetics to be easily implemented in the plug-flow reactor specifications and can be accepted when considering the relatively small dimensions of coal particles (100 μm).

The gasification block is modeled assuming a temperature profile on the basis of reference data on a similar reactor.²⁰ Data were available only for a peak temperature of approximately 1450 °C. For different peak temperatures, the profile is adapted (Figure 3) from the available data by a function in the AspenPlus Calculator. This procedure allows the actual gasification profile to be determined once the design specification is solved giving the peak temperature.

3.5. Quench Section. In the bottom part of the gasifier, the syngas and the solid residues are cooled down by quench water and cooling jacket, which produces hot pressurized water. This final step is schematized in three stages to avoid an instantaneous evaporation of the global water added. Each stage is formed by a mixer block, representing one-third of the overall quench water, and a heater block, representing the heat recovery of the cooling jacket. It is worth noting that these blocks ensure an equilibrium between liquid and vapor phases.

The exit temperature of the syngas is fixed to 200 °C and is guaranteed by a design specification which finds the corresponding value by varying the overall quench water. In all cases, the water-to-coal ratio is maintained in the range 0.10–0.20 wt/wt.

Finally, 90% of the solid (ash or residual char) in the syngas is assumed to be removed as slag. Some soluble components are also removed in the wastewater. The distribution is calculated on the basis of equilibrium between liquid and vapor phases in heater and mixer blocks.

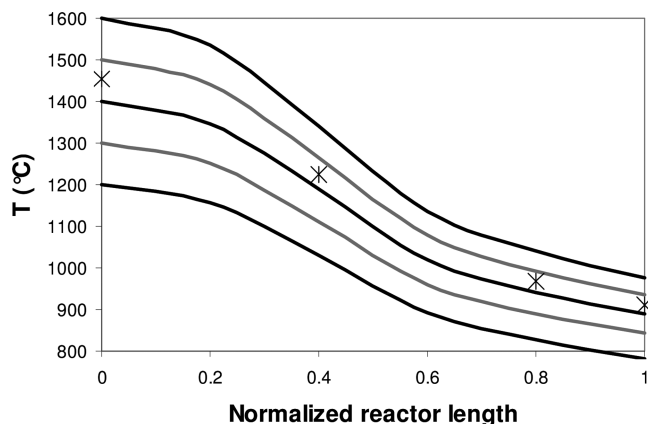


Figure 3. Assumed thermal profile inside the reactor (top section). Symbols represent reference data.²⁰

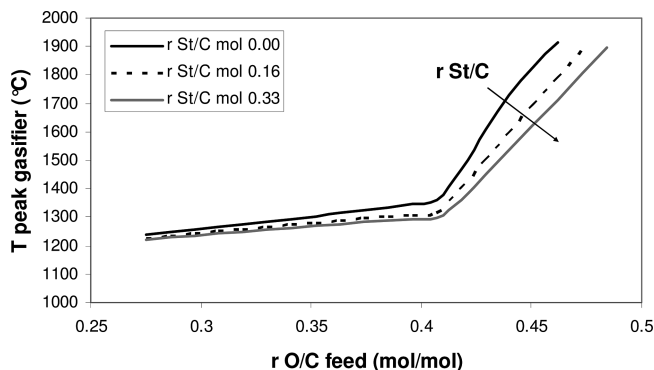


Figure 4. Peak temperature calculated as function of the oxygen-to-carbon ratio at various steam-to-carbon ratios.

4. Results

4.1. Parametric Analysis. The effects of the operating conditions on the syngas conversion are evaluated to optimize the gasifier performance. The fuel feed is maintained constant in all simulations, while the oxygen-to-carbon (rO/C mol/mol) and steam-to-carbon (rSt/C mol/mol) ratios are varied in wide ranges (0.25–0.50 and 0.15–0.35, respectively). Also, the case of no steam added to the gasifier is considered to quantify the importance of steam gasification to the gasifier performance. In this case, some water is actually present in the reactant gas due to the evaporation of the fuel moisture and also as a product of primary pyrolysis.

In general, the higher rO/C, the higher the temperature in the reactor (a limit for the parametric analysis is fixed for peak temperature of 2000 °C). This is due to the higher conversion of combustion reactions. The results of the model on the peak temperature are reported in Figure 4. For the case under study, a critical point can be observed for rO/C around 0.41: under this point, the temperature increases slowly with rO/C and the effect of rSt/C on the temperature is small; the temperature ranges between 1200 and 1300 °C. At the critical point, the temperature is approximately 1300 °C for the value of rSt/C 0.25. A significantly higher temperature (1360 °C) is reached in the case of no steam added to the gasifier. It is worth noting that temperatures higher than 1200 °C are crucial for this kind of gasifiers to melt and remove the ash in the slag and minimize the formation of tar.

Above the critical point, the temperature increases quickly and the effect of rSt/C is more pronounced: the higher rSt/C, the lower the temperature and the more favored the gasification reactions.

These results can be explained when considering the syngas composition as in Figure 5 for the value of rSt/C 0.25 taken as reference. For rO/C values lower than 0.41, the char conversion is not complete and a significant amount of tar and CH_4 can be observed. At the critical point, the temperature of 1300 °C is high enough to consume the char (partially by combustion, mostly by gasification). Above this point, the “excess” oxygen consumes the most reactive products, i.e. H_2 and CO , with an increase in the combustion products, H_2O and CO_2 , respectively. This makes the temperature to increase significantly, but a lower production of hydrogen can be observed. So a high temperature is not suitable for maximizing hydrogen production. Furthermore, a high temperature would jeopardize the materials.

The maximum in the hydrogen production varies also with the steam-to-carbon ratio (Figure 6). At rSt/C 0.25, it is achieved at rO/C 0.42 and corresponds to 0.48 mol H_2 /mol C in the feed. Considering that the downstream units of a gasification process

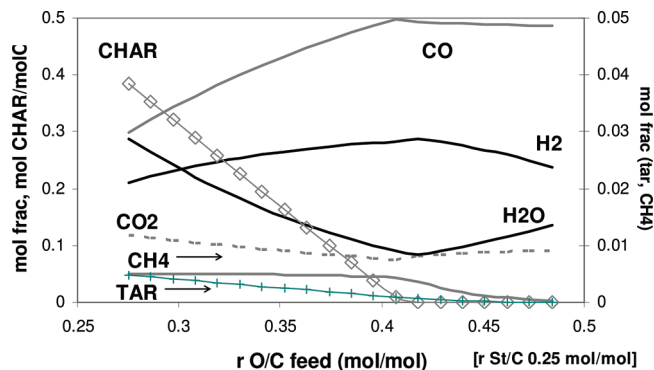


Figure 5. Syngas composition and char conversion calculated as function of the oxygen-to-carbon ratio.

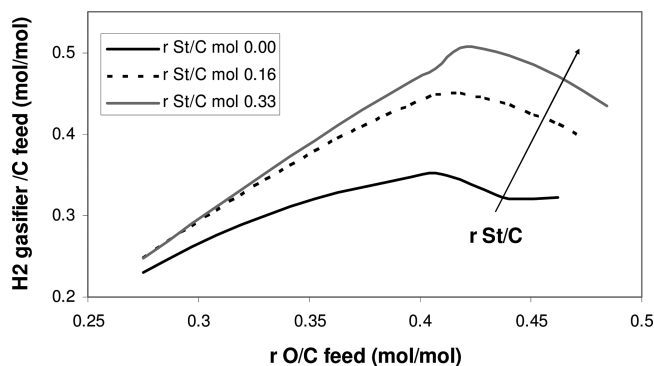


Figure 6. Hydrogen production calculated as function of the oxygen-to-carbon ratio at various steam-to-carbon ratios.

will convert the CO with a water–gas shift reaction, also the production of CO is important. At rSt/C 0.25, the maximum is reached at rO/C 0.41 and is 0.83 mol CO/mol C in the feed.

Vice versa, CH_4 formation represents a loss in the efficiency and is always under 0.006 mol CH_4 /mol C above the critical point. Tar is calculated to be 0.001 mol TAR/mol C at the critical point and then decreases rapidly to negligible values.

4.2. Comparison of Model Results with Equilibrium Results. An RGibbs reactor (an equilibrium reactor model, which minimizes the free energy in AspenPlus) is used in the reference conditions to substitute the entire scheme of the gasifier model described above. The equilibrium results on the main gaseous products (CO, CO_2 , and H_2) in the syngas agree with those of the gasifier model for gasification temperatures between 1000 and 1400 °C. This is obvious when considering that this gasifier allows to approach the equilibrium.

However, as reported in the introduction, some problems arise for an optimization study. First of all, the temperature should be fixed a priori, and the definition of the representative value might be arguable. The maximum temperature is hardly suitable, being reached only in a small zone of the gasifier. An average temperature of the entire profile may underestimate the yield of faster reactions. The gasification temperature could be even considered as a “fit parameter” to match the syngas composition (as in the restricted equilibrium models related to global and individual reactions²²), but this would reduce the predictive ability of the model. Furthermore, a temperature range between 1000 and 1400 °C is too wide for a reliable analysis. So, the recommendable solution is to relate the temperature to the operating conditions and obtain it from a heat balance on the entire reactor, as discussed in this work.

Second, tar and residual char calculated from an RGibbs reactor are negligible for all conditions of temperature and

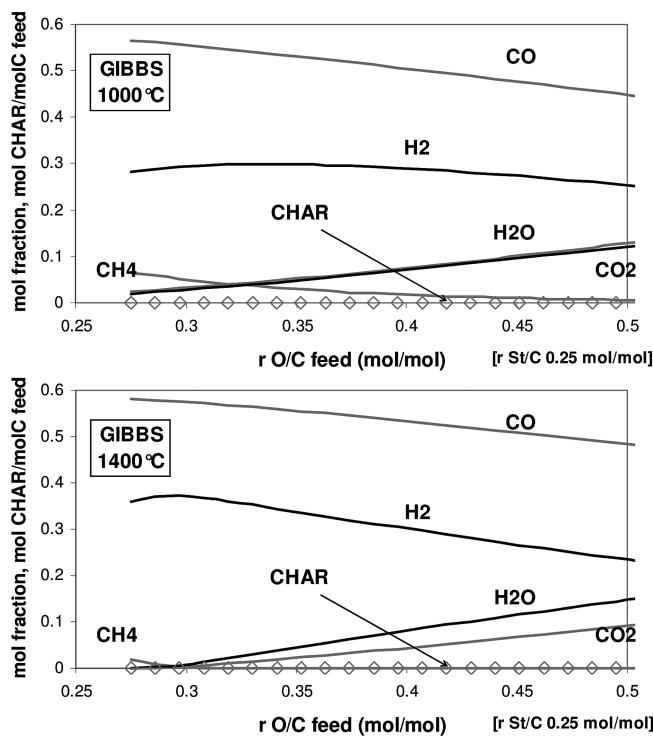


Figure 7. Syngas compositions calculated by using an RGibbs reactor at various temperatures.

oxygen-to-carbon ratio studied (Figure 7). This is unrealistic and may lead to unsuitable conditions of optimization. Conditions of hydrogen maximization are far from those evaluated by a more detailed approach. Finally, heat recovery cannot be quantified.

4.3. Comparison of Model Results with Experimental Data and Discussion. The results of the analysis described in this work can suggest the optimal conditions for maximizing the hydrogen production. An optimization efficiency should be actually defined, because many targets can be pursued. The gasifier will be connected to other units that can increase the hydrogen production via CO shift, so that the operating conditions can be chosen to maximize the final hydrogen production. Also, steam and oxygen consumption will affect the energetic and economic efficiency of the gasifier or the hydrogen production plant. Heat recovery and integration can improve this efficiency. The maximum temperature arisen may be a constraint for the materials used in the reactor, so it should be taken into account when studying the optimization of the process. Also, tar or pollutant removal should be evaluated as a function of the operating conditions.

In all cases, the implementation of the gasifier model described in this work in a comprehensive process model represents an effective tool for studying the optimization of hydrogen production, giving the syngas composition in terms of main gaseous species (H_2 , CO, CO_2) as well as “byproducts” (CH_4 , tar). The separation of main steps allows the heat balance to be solved and gives the gasification temperature as a function of the operating conditions (rO/C and rSt/C). It also quantifies the heat recovery for the production of steam.

Syngas composition calculated under the optimal conditions agrees with data reported by producers. In this case, the steam-to-carbon ratio is 0.25. The maximum temperature recorded in the gasifier is around 1400 °C, while the calculated peak temperature in the same conditions is 1380 °C. The agreement based only on the main gaseous species is very good (see Figure

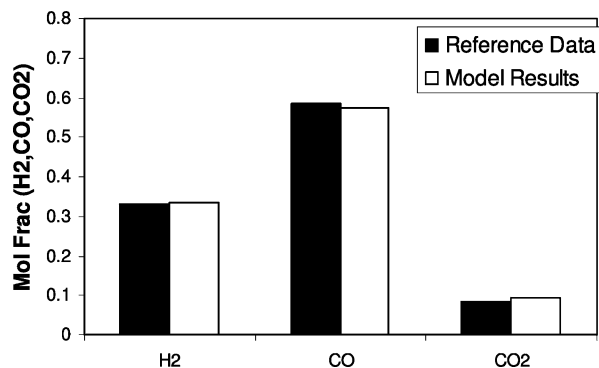


Figure 8. Comparison of gasifier model results with reference data. Model results: rO/C 0.418, rSt/C 0.25.

8) for the molar fraction of hydrogen, CO, and CO₂. Also the results on the CH₄ yield is in agreement (mole fraction of approximately 1% as observed in Figure 5). Finally, the carbon conversion (evaluated as the nonconverted char and tar) is greater than 99% in the operated range of temperature. This set of results (temperature, syngas composition, and heat recovery, which was modeled according to the preliminary reactor size) demonstrates the validity of the model proposed.

5. Conclusions

An entrained flow gasifier model was developed by using AspenPlus. The target was a tool for optimization studies to be implemented in a comprehensive process model for the production of hydrogen via coal gasification. It was developed as a multizonal model by modeling each step of the gasification (preheating, devolatilization, combustion, gasification, quench) according to the reactor configuration, that is an entrained flow reactor. In this way, the temperature could be related to the operating conditions, i.e. fuel, oxygen, and steam flow rates. This aspect is valuable in itself because it removes the hypothesis of equilibrium reactors which required a fixed temperature of gasification. Furthermore, the heat balance on the entire reactor is allowed to quantify the heat recovery, which could be crucial for efficiency calculations of the hydrogen production plant. Also, byproducts and residual char could be quantified and minimized based on the operating conditions. Finally, in view of future works, the development of a gasifier model (with the possibility to insert design parameters) instead of a gasification model will allow different reactor configurations to be compared (fixed beds, fluidized beds, entrained flow reactors) by adapting the procedure to other systems.

Acknowledgment

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