Research Article

Thermochemical Equilibrium Model of Synthetic Natural Gas Production from Coal Gasification Using Aspen Plus

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The production of synthetic or substitute natural gas (SNG) from coal is a process of interest in Colombia where the reserves-to-production ratio (R/P) for natural gas is expected to be between 7 and 10 years, while the R/P for coal is forecasted to be around 90 years. In this work, the process to produce SNG by means of coal-entrained flow gasifiers is modeled under thermochemical equilibrium with the Gibbs free energy approach. The model was developed using a complete and comprehensive Aspen Plus model. Two typical technologies used in entrained flow gasifiers such as coal dry and coal slurry are modeled and simulated. Emphasis is put on interactions between the fuel feeding technology and selected energy output parameters of coal-SNG process, that is, energy efficiencies, power, and SNG quality. It was found that coal rank does not significantly affect energy indicators such as cold gas, process, and global efficiencies. However, feeding technology clearly has an effect on the process due to the gasifying agent. Simulations results are compared against available technical data with good accuracy. Thus, the proposed model is considered as a versatile and useful computational tool to study and optimize the coal to SNG process.

1. Introduction

Coal is a major source of energy, accounting for ~25% of the world energy supplies and ~40% of the world electricity generation. It is predicted that coal will continue to play an important role in meeting the world's increasing energy demands in the foreseeable future [1]. However, the use of coal faces several challenges such as clean and efficient energy systems, the challenge of carbon storage and sequestration, and the environmental impacts due to the mining [1, 2]. The coal gasification in entrained flow reactors with steam and/or oxygen produces synthesis gas (syngas), which is a mixture of mostly hydrogen and carbon monoxide [3]. Therefore, the urgent needs to produce fuels and chemical products from syngas prompt the study of this thermochemical process [3, 4]. Gasification units in electric power plants produce a fuel gas to drive gas turbines. And gasification in chemical plants yields syngas that can be used to produce a wide spectrum of chemical products, such as ammonia, methanol, methane, and liquid fuels [5]. Future plants will be hybrid power/chemical plants with gasification as the key unit operation; as a consequence, the thermochemical process has been emerging as the premier unit operation in the energy and chemical industries. Therefore, the gasification continues to be an important topic to research [3, 6, 7].

The production of SNG from coal is a process of particular interest to Colombia, where depletion of natural gas is being foreseen in the coming years due to the increasingly high level of demand of the last several years [8]; carbon reserves are still foreseen to last for around 90 years [9, 10]. These reserves are the highest coal reserves in South America. The coal production in Colombia is distributed by

regions as follows: 50.92% Cesar, the main coal mines are *El Descanso*, *Calenturitas*, *La Loma*, and *Jagua*; 38.87% La Guajira (*Cerrejón* coal mine); 3.57% Cundinamarca (*Guaduas* coal mine); 3.21% Boyacá (*Tunja-Duitama*, *Sogamoso-Jericó*, and *Chinavita-Umbita-Tinabá* coal mines); 2.22% Norte de Santander (*Zulia*, *Cúcuta*, *Tasajero*, and *Toledo* coal mines); and 1.21% others. Therefore, one of the main challenges facing the country is finding how to add value to mineral resources under environmental, efficiency, and sustainability criteria [1]. Therefore, this study is focused on modeling the SNG production process by means of coal gasification in entrained flow as a promising and clean alternative way to produce energy and fuels.

Several studies of modeling coal gasification have been published in the specialized literature. Gräbner and Meyer [11] analyzed the gasification process under the first and second thermodynamic laws. The aim has been to study the coal rank effect (standard and high ash content coals) on the gasifier technology (Shell, Siemens, Texaco, ConocoPhillips, and High Temperature Winkler-HTW). The higher exergy efficiencies were reached by slurry feeding and dry feeding technologies with the standard coal.

Kunze and Spliethoff [12] developed a model with Aspen Plus to simulate a generic entrained flow gasifier. The objective was to analyze the effect of the fuel feed system, that is, dry feed and slurry feed on the gasification process at 30 bar. They found higher energy efficiency for dry feed gasification (83%) when compared with slurry feed (72%). Seifkar et al. [13] studied the effect of coal supply and reactor cooling system on the entrained flow gasifier process. They analyzed three systems: the first one included dry coal feed and reactor cooling with water, the second consisted of one dry coal feed with partial cooling with water, and the last one was a coal slurry feed supply system without refrigeration. The authors discussed advantages and disadvantages associated with the studied systems.

Maurstad et al. [14] presented a model with Aspen Plus to characterize an integrated gasification combined cycle plant (IGCC) with and without CO_2 capture. They carried out a comparison between two technologies (dry feed and slurry feed) with five types of coal in the IGCC plant energy behavior. They found that the thermal efficiency and power of the IGCC plant diminished with the coal rank for the slurry feed technology, while the dry feed technology was not affected. Yu et al. [15] studied the effect of the gasification technology on the water gas shift reaction unit used for Fischer-Tropsch processes. The study was conducted by means of an Aspen Plus model. They showed that the dry feed technology presented higher energy efficiency and lesser H_2/CO ratio with regards to the slurry feed technology. Prins et al. [16] studied different ways of carbon capture and sequestration on an IGCC plant by process modeling. The dry feed technology was analyzed because of its higher efficiency in the gasification process (82.3%) against the gasifiers with slurry feeding systems (about 75%).

Bockelie et al. [17] studied the syngas composition and the cold gas efficiency of two commercial gasifiers using a computational fluids dynamic model (CFD). The commercial gasifiers considered were Shell (dry feed technology with one gasification stage) and ConocoPhillips (slurry feed technology with two gasification stages). The authors highlight the agreement between the simulation results with the proposed model and the data reported in the literature. Armin [18] and Silaen and Wang [19] conducted numerical simulations of the gasification process in entrained flow reactors. They studied the effect of the operating parameters such as coal dry feeding and slurry feeding systems, type of gasifying agent, and coal rank in the global gasifier performance. They highlighted that syngas heating value (HHV_{syngas}) is higher with the dry system technology. Moreover, the carbon conversion efficiency and HHV_{syngas} increase when oxygen is used as gasifying agent because the nitrogen inert effects of the air are avoided.

Using biomass as a feedstock to produce SNG by means of gasification, Vitasari et al. [20] developed an Aspen Plus model to conduct an exergy analysis of different biomass types (wood, urban solid wastes (USW), and sewage sludge). They simulated the process under different operating conditions, including variations in the reactor pressure as well as temperature and pressure in the methanation reactor. The global process exergy efficiency was reached with wood being between 53 and 58%; for USW was between 42 and 46% and for the sewage sludge being from 47 to 57%. Tremel et al. [21] simulated a small scale plant to produce SNG via indirect steam biomass gasification. The thermal biomass input to the gasifier was 500 kW. The model was developed under equilibrium approach using Aspen Plus and considering the minimization of the Gibbs free energy. They studied the effect of four operation conditions on the energy efficiency of the process. The ratio between the energies of SNG and biomass reached values around 66–75%. This indicator increases when the pyrolyzed char is used to feed the steam boiler.

Heyne et al. [22] studied the thermal integration between an existing biomass steam and power cycle (CHP) and the production process of SNG via indirect gasification. The thermal plant was modeled and simulated by means of Aspen Plus, and the analysis was conducted using pinch technology. The process global efficiency reached was about 90%, and it indicates that the SNG production is feasible via indirect gasification coupled to a CHP plant.

On the other hand, the Department of Energy from the United States through the National Energy Technology Laboratory conducted a diagnosis of commercial entrained flow gasifiers. The analysis was carried out by means of Aspen Plus models and validated with data from 14 IGCC plants. The IGCC plants efficiencies without CO_2 capture were 42.1%, 39.7%, and 39% for Shell, ConocoPhillips, and Texaco, respectively. Regarding the costs, the specific costs of the IGCC plants without CO_2 capture were about 2350 $USD/kW for ConocoPhillips (slurry feed technology) and 2710 $USD/kW for Shell (dry feed technology) [23].

The coal gasification process has been widely studied under different operational conditions. This has been done by means of modeling and simulation strategies with software tools such as Aspen Plus to analyze the thermochemical process or to study how the input parameters affect the IGCCs process. According to the literature cited, the effect of coal gasification technology on the SNG production using

Aspen Plus model has not been presented. Therefore, in the current study, two typical technologies used in entrained flow gasifiers with dry coal and slurry coal feed systems are modeled and simulated. Emphasis is put on interactions between the fuel supply technologies and energy output parameters of coal-SNG process, including carbon conversion efficiency, cold gas efficiency, process and global energy efficiencies, SNG heating value, Wobbe Index, and power. Since most of the revised literature did not go deep into model details, this study presents as an additional contribution, a comprehensive and complete model of coal to SNG process under thermochemical equilibrium developed in Aspen Plus.

2. Methodology

*2.1. Coal-SNG Process Description: Coal Slurry Feed Mode.* The complete process to produce SNG via coal gasification in entrained flow reactors with slurry feeding system includes several stages that are shown in Figure 1. Stage 1 includes the solid fuel inlet into the system as a slurry after mixing it with water. The typical concentration of water in the slurry is around 30–40% wt., which means that a significant portion of heat generated by coal combustion will be used to vaporize water in the gasifier at higher pressure. Therefore, the cold gas efficiency (CGE) of wet feed gasifiers is expected to be lower (between 8 and 10%) than the dry feed gasifiers [12, 16].

The entrained flow gasifier is modeled with two gasification stages, 70% of slurry mass flow goes into a pressurized reactor (Stage 2, Figure 1) where the slurry reacts with oxygen (98% purity). The use of air as an oxidant is avoided due to high flow rates that produce stack gas by the higher amount of nitrogen. The syngas formed in this reactor flows to a second pressurized reactor (Stage 3, Figure 1) where reaction takes place with the remaining 30% of the initial slurry mass flow. In the second reactor, there is not an addition of oxygen. In this way, the coal devolatilization is promoted and the reduction reactions for CO_2, H_2, and H_2O with char are driving to formation of H_2, CH_4, and CO as majority compounds, (1)–(3). Consider

$$C + CO_2 \Longleftrightarrow 2CO \tag{1}$$

$$C + 2H_2 \Longleftrightarrow CH_4 \tag{2}$$

$$C + H_2O \Longleftrightarrow CO + H_2 \tag{3}$$
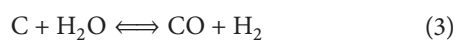
The units downstream from the gasifier are mostly standard gas-phase processes [3]. Syngas produced in the gasification process (Stage 2-3, Figure 1) goes through a separator that removes unreacted coal (Stage 4, Figure 1). Unreacted coal is reentered to the process as recycled char in Stage 1. Further, in Stage 5 (Figure 1) the syngas is quenched and cooled with water with the corresponding ash solidification (slag formation). The slag is removed from the syngas in a particulate removal system. According to the particle size distribution, the particulate matter clean-up process can include cyclones, electrostatic precipitators, and bag filters. After cooling and particulate removal, the syngas is fed into a water gas shift reactor (WGSR), where hydrogen formation is promoted (Stage 6, Figure 1). By adding steam

to the WGSR, carbon monoxide and water react to carbon dioxide and hydrogen (see (4)). In this way, the WGSR can produce a modified syngas with specific molar ratio H_2/CO by adjusting any of the reactor inlet flows (steam and/or syngas). Consider

$$CO + H_2O \Longleftrightarrow CO_2 + H_2 \tag{4}$$
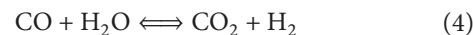
The molar ratio H_2/CO at the exit of the WGSR will depend on aims of the entire plant process; that is, for dimethyl synthesis, a molar ratio $H_2/CO = 1$ is desired, while Fischer-Tropsch process requires a ratio $H_2/CO = 2$. For SNG production, a molar relation $H_2/CO = 3$ is preferred [21, 24, 25]. Thereby, a portion of the syngas from Stage 5 (Figure 1) is bypassed and only between 60% and 70% of the syngas mass flow goes through the WGSR. In chemical applications, the synthesis gas and/or hydrogen is fed to downstream chemical plants. The carbon dioxide is suitable for sequestration [3], or it can be also used as a carrier gas in entrained flow gasifiers with dry feeding technologies [12]. In the SNG production scheme (Figure 1), the syngas with adjusted-molar ratio H_2/CO is then passed through an acid gases recovery unit (AGR), which consists of a separation unit that removes acid gases (Stage 7, Figure 1). In the AGR unit the syngas is cleaned up from acid gases and other impurities that are formed upstream in the process, such as NH_3, HCl, H_2S, COS, H_2O, and CO_2, among others. This cleaning process is necessary because the next process stage (Stage 8, Figure 1) consists of a catalytic reactor whose performance highly depends on the quality of the reactor inlet gases [24]. Furthermore, in the reducing environment present in gasifiers, the sulfur and nitrogen impurities appear as hydrogen sulfide and ammonia, respectively. Both of these chemicals can be easily removed using pollutant removal systems (i.e., sulfur dioxide absorbers and NOx reactors) and are potentially valuable by-products to be used as well or as raw material for different chemical process, that is, a sulfuric acid plant production. In the current process, the outcoming gas from Stage 7 (Figure 1) is constituted mainly by H_2 and CO. This syngas with adjusted-molar ratio $H_2/CO = 3$ flows to the methanation stage (Stage 8, Figure 1) where methane formation is promoted (see (5)). Even when additional reactions could occur in the methanation reactor, that is, (6), the methane formation by (5) is thermodynamically favored due the operating conditions in the reactor (temperature and pressure) as well as the composition of the reactor inlet gases and the adapted catalytic technology. Simulations in this study revealed that, under the conditions given, the equilibrium constant of the reaction presented in (6) is 22 times lower than equilibrium constant of the reaction presented in (5). Thus, there are no significant errors in assuming (5) as the only reaction taking place on the methanation reactor.

Stage 9 (Figure 1) corresponds to the SNG conditioning stage. The SNG is cooled; therefore, steam formed in Stage 8 (see (5)) is condensed and separated from the SNG. The outlet of this block (Stage 10, Figure 1) corresponds to the desired
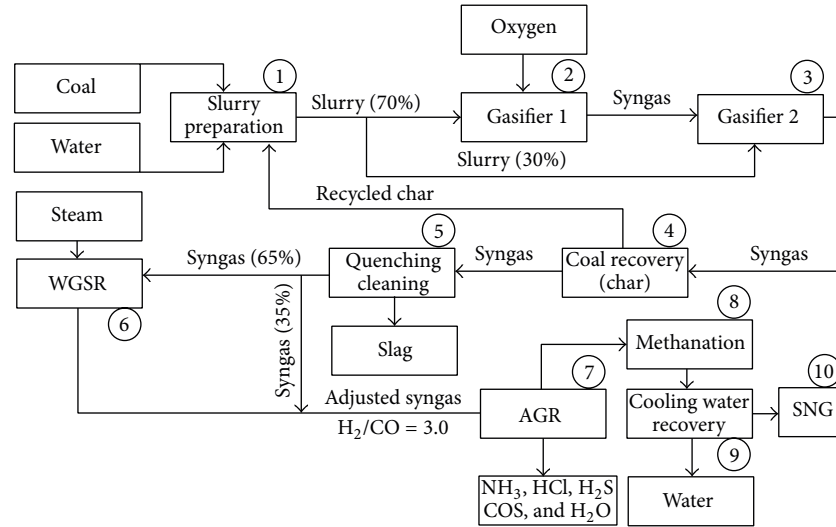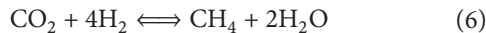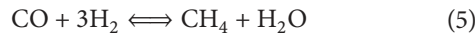
FIGURE 1: Process stages of SNG production via coal gasification using slurry feeding technology.

natural gas at temperatures around 50–60°C with high level concentrations of methane (SNG). Consider

$$CO + 3H_2 \Longleftrightarrow CH_4 + H_2O \quad (5)$$

$$CO_2 + 4H_2 \Longleftrightarrow CH_4 + 2H_2O \quad (6)$$

2.2. Coal-SNG Process Description: Dry Coal Feed Mode. The process diagram to produce SNG via coal gasification using an entrained flow reactor with dry feeding technology is presented in Figure 2. Stage 1 represents the fuel inlet to the system mixed with CO_2 in an entrained flow gasifier. It should be noted that compared with the slurry feeding technology, this process require that the coal goes to the gasifier with very low moisture content, between 1% and 2%. In the dry feeding technology, the gasifier includes just one reactor [26] (Stage 2, Figure 2). All remaining stages in the dry feeding technology correspond to the analogous stages that were described in the slurry feeding technology (Section 2.1). However, the amount of syngas that passes through the WGSR is different for both technologies. In the dry feeding technology, around 85%–95% of the syngas mass flow goes through the WGRS and the remainder of the syngas is bypassed to acid gases recovery unit (AGR). This is because the syngas molar ratio CO/H_2 leaving the gasifier in slurry technology is around 1 : 1, while in dry technology the syngas CO/H_2 molar ratio is around 2 : 1. The higher CO concentration in the syngas leaving from the gasifier with dry feeding technology is attributed to the lower amount of water in the gasification process, which is directly related with the H_2 concentration.

2.3. Test Fuels. The chemical characterization of the Colombian coals used in this study is presented in Table 1. According to the ASTMD88-12 standard, the Sanoha coal is classified as bituminous coal and Bijao coal is a subbituminous type B coal. These fuels are used to validate the model with technical data.

TABLE 1: Chemical characterization of Colombian coals (Bijao coal and Sanoha coal) used in simulations.

Characterization	Bijao	Sanoha
Proximate analysis (wt.% wet)		
Ash (ASTM D 73174)	6.5	14.8
Volatile matter (ASTM D 3175)	45.89	29.85
Fixed carbon (ASTM D 3172)	47.61	55.35
Moisture content (ASTM D 3302)	19.05	4.93
Ultimate analysis (wt. % dry)		
C	68.24	72.11
H	4.9	4.78
N	1.59	1.62
S (ASTM D 5865)	1.36	1.44
O	17.38	5.52
Cl	0.03	0
Ash (ASTM D 73174)	6.5	14.8
$HHV_{d.b}$ (kcal/kg) (ASTM D 5865)	5407	7538

2.4. Software Selection. Simulations were carried out using Advanced System for Process Engineering simulation software (Aspen Plus v7.3) [27]. Aspen Plus is a process modeling software suitable for a variety of steady state modeling applications. Currently, this software was widely applied in simulating gasification processes, cogeneration plants, and polygeneration systems, all of them with different technologies and fuels [12, 28–34], and good agreement between the industrial data and those determined using the Aspen models was obtained [35, 36]. Aspen Plus software provides a flexible input language for describing the SNG production process, including its components, connectivity, and computational sequences. Use of Aspen Plus leads to an easier way of model development, maintenance, and updating since small sections of complex and integrated systems can be created and tested as separate modules before they are integrated. It
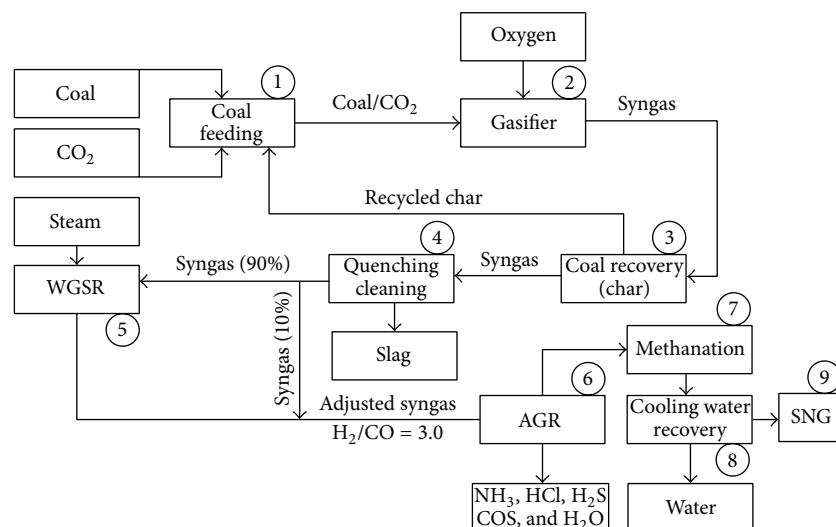
FIGURE 2: Process stages of SNG production via coal gasification using dry feeding technology.

has an extensive physical properties database to model the material streams in SNG production process [6, 30, 33, 37, 38]. Additionally, Aspen Plus has many built-in model blocks (such as heaters, pumps, stream mixers, and stream splitters), some of which can be directly used in this work.

3. Aspen Plus Model Description

3.1. Hypothesis. The relatively high temperatures used in the gasification process allow the consideration that the kinetic barriers are minimized and it was found that the gaseous mixtures leave from the gasifiers approach to the equilibrium [4, 39]. Therefore, the gasification process can be successfully described by means of a thermodynamic model [27, 40]. In this work, an overall equilibrium approach is employed while neglecting the hydrodynamic complexity of the gasifier. Other assumptions in the model are: (1) stationary state, (2) WGSR and methanation reactor which are equilibrium-isothermal reactors, (3) char which is supposed to be 100% graphite (conventional substance available in Aspen Plus database), (4) the ash content which is turned into slag, and (5) the gasifier reactors which are simulated as RGibbs adiabatic reactors. In addition, the conditioning coal (drying) and air separation unit to get oxygen as a gasifying agent are not considered in the model.

The RGibbs reactor was chosen because this kind of reactor can handle three phases under chemical equilibrium and allows predicting the equilibrium composition of the produced syngas by minimizing the Gibbs free energy [21]. Indeed, the RGibbs reactor of Aspen that works under the Gibbs free energy minimization principle has been widely adopted to represent gasification reactions [6, 41–43]. The equilibrium products potentially formed in the RGibbs reactors are H_2O, N_2, O_2, H_2, C, CO, CO_2, CH_4, H_2S, NH_3, COS, HCl, and Cl_2 [24, 28]. These species allow the versatile simulation of different kind of syngas, depending on the input parameters. Definition of species potentially formed in the

gasifier was based on the following considerations. (i) CH_4 is the only hydrocarbon taken into consideration in this work due to higher pressure and temperature [4]. (ii) The sulfur contained in the coal is assumed to be converted mainly into H_2S and COS. The low amounts of chlorine suggest that the chlorinated species formed are only traces of HCl and Cl_2; and (iii) the assumption that only NH_3 forms and not oxides of nitrogen are produced has already been made by other researchers [44].

3.2. Coal to SNG Model. This section discusses how Aspen Plus is used to simulate the SNG production via coal gasification using slurry feeding technology. Also, the main differences are described in the modeling approach for dry feeding technology. The Aspen Plus process flow sheet is divided into five hierarchies (Figure 3): slurry preparation (FEEDING), gasification (GASIFIC), water gas shift reactor (SHIFTING), acid gas recovery unit (AGR), and methanation (METHANAT). Each one of these hierarchies includes at least one Aspen Plus built-in block, and in some cases, that is, in the FEEDING hierarchy, there are also included additional Fortran subroutines.

In the case of dry feeding technology, the main process diagram is quite similar to the one shown in Figure 3. In the flow sheet of the dry feeding technology, the WATER inlet stream is replaced by a CO_2 inlet stream. Differences between the models of both feeding modes are appreciated inside some specific hierarchies that are described below.

3.2.1. FEEDING Hierarchy. The Aspen Plus model used for simulating the slurry preparation (FEEDING hierarchy) is showed in Figure 4.

FEEDING hierarchy (Figure 4) is used to simulate the raw material inlet to the process (Stream COAL) which is composed only by coal as received in the plant; that is, neither crushing processes nor drying processes are considered. The feedstock is Colombian coal with the proximate analysis and
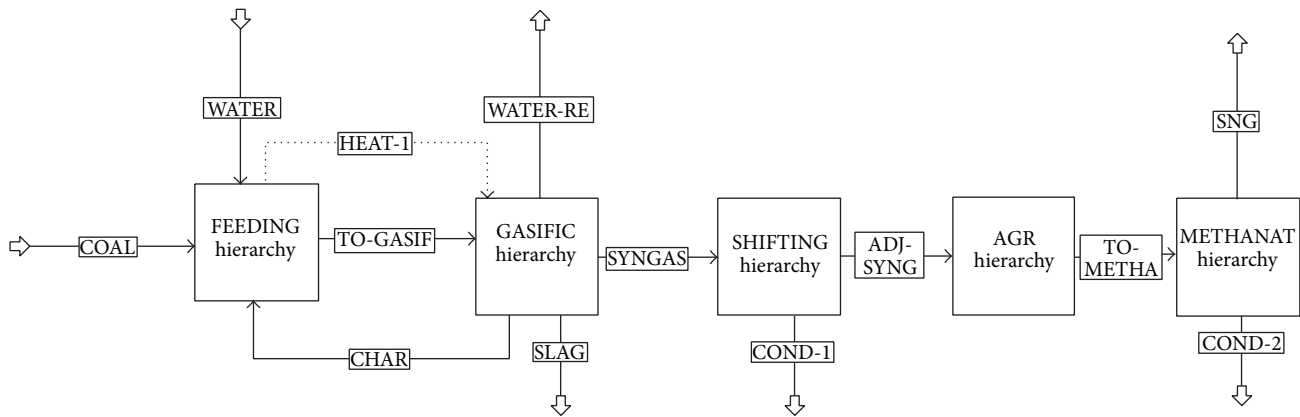
Figure 3: Aspen Plus process flow sheet for SNG production via coal gasification using slurry feeding technology (ConocoPhillips 66).
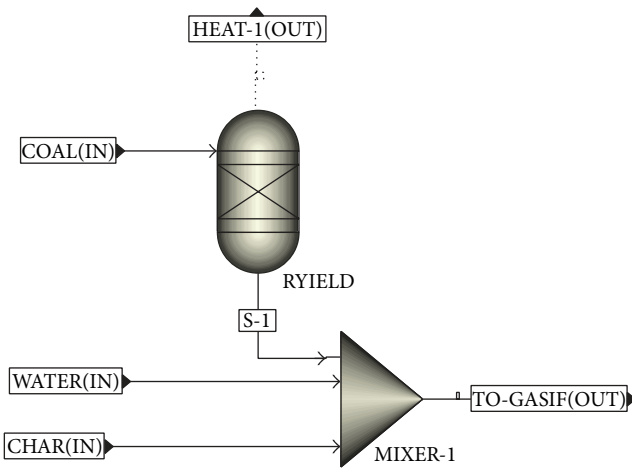

Figure 4: Aspen Plus feeding hierarchy for the simulation of the slurry preparation in the SNG production via coal gasification.

ultimate analysis given in Table 1. Aspen Plus cannot handle nonconventional substances, and coal is a nonconventional solid with a complex macromolecular structure [45, 46]. Therefore, the coal stream needs to be hypothetically decomposed in reactive compounds, that is, its corresponding constituents (such as C, H_2, N_2, O_2, S, Cl_2, and H_2O), based on its proximate analysis and ultimate analysis. This is performed in a yield reactor (RYIELD block, Figure 4) [41, 43–46]. The yield distribution for this reactor has been specified by FORTRAN statements in a calculator block [47]. These statements specify the mass flow rates of the components in the stream S-1, Figure 4. The slurry is then formed by mixing the stream S-1 with the inlet stream WATER in the mixer block MIXER-1, and it is driven to the next process stage through the stream TO-GASIF (Figure 4). The stream TO-GASIF leaves from the FEEDING hierarchy and becomes the main inlet to the GASIFIC hierarchy, where the formation, quenching, conditioning, and cleaning of the syngas are simulated. In the built-in mixer block (MIXER-1), the unreacted solid coal (char) from the gasification process stage is reentered to the process. By the other side

regarding the energy, the heat of reaction associated with the coal decomposition is carried by the heat stream HEAT-1 (Figure 4) into the next hierarchy (GASIFIC, Figure 3) [25, 30], where gasification reactions have been modeled [47]. Then, further gasification reactions were applied to the available constituents of the coal at the same enthalpy level.

When dry feeding technology is simulated, the Aspen Plus flow sheet for FEEDING hierarchy is quite similar to that described in Figure 4; the only difference is the use of a CO_2 inlet stream instead of the WATER inlet stream, taking into account the lower moisture content of the raw material (1%-2%).

3.2.2. GASIFIC Hierarchy. Figure 5 is a schematic diagram of the Aspen Plus model for the gasifier facility [48, 49]. The gasification facility consists of three sections: a reactor, quenching, and cleaning systems (solids and liquid removing from the syngas). In the modeled slurry technology, the gasification system is comprised of two RGibbs reactors (RGIBB-1 and RGIBB-2, Figure 5). The stream TO-GASIF coming from FEEDING hierarchy is split into two streams by a stream divisor block (SPLIT1). The formed streams S-2 and S-3 (Figure 5) carry on the 70% wt. and 30% wt. (resp.) of the total material coming in the stream TO-GASIF. In the same way, the heat stream HEAT-1 is divided in two heat streams H-2 and H-3 with a stream divisor block (QSPLIT), Figure 5. The stream S-2 reacts with the inlet stream OXYGEN in the RGIBB-1 reactor. The mass flow of the OXYGEN stream can be adjusted in order to modify the equivalence ratio (ER) (see (7)) or the reactor temperature. The stream S-4 (Figure 5) feeds the second RGibbs reactor RGIBB-2 and reacts with the stream S-3. In this way, the formation of H_2, CH_4 and CO is promoted; see (1)–(3). The stream S-5 (Figure 5) is then quenched and cooled by mixing it with water from the inlet stream WATQFEED in the Aspen Plus built-in blocks MIXER-2 and HEATER-1. The next step is the block SSPLIT, it is used to simulate a stream divisor. SSPLIT is an Aspen Plus built-in block that allows completely separating conventional from no conventional compounds as well as solids from liquids and gases. Thus, the SSPLIT separates conventional solids and unconventional solids and the gaseous phase
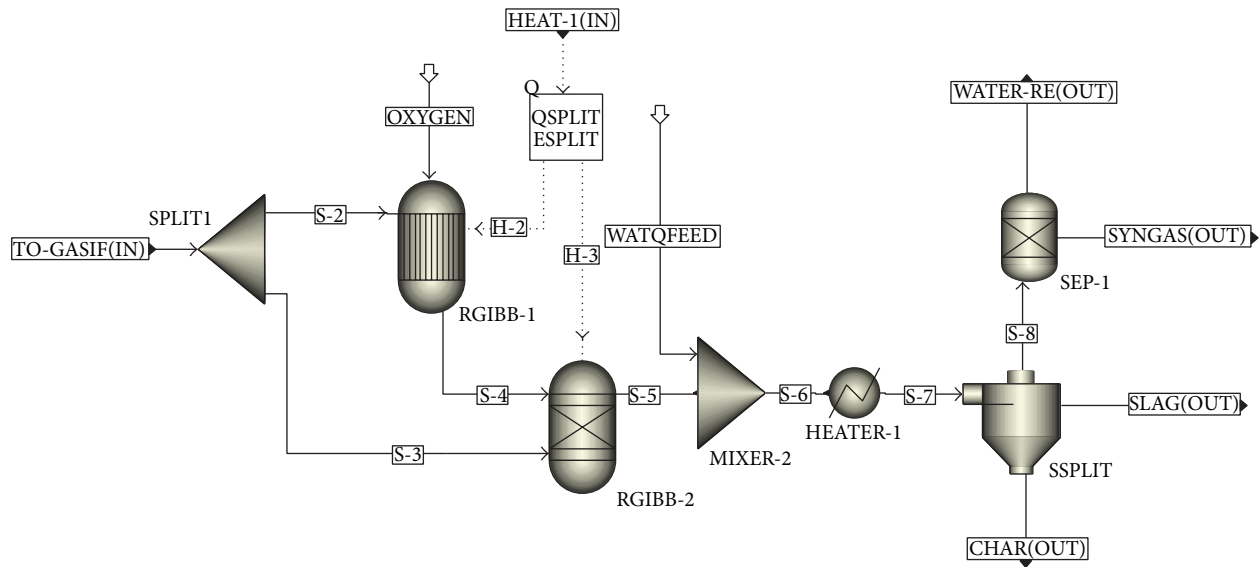
FIGURE 5: Aspen Plus GASIFIC hierarchy diagram to simulate the gasification stage of coal-SNG process. Flow sheet for the slurry feeding technology.

coming from the reactor [6, 47]. The conventional solids correspond to the unreacted coal or char (stream CHAR), and the unconventional solids are mainly ash (stream SLAG). Stream CHAR is recycled and fed back into the process in the FEEDING hierarchy; in contrast, the stream SLAG is discharged from the process. The remaining wet gaseous mixture (stream S-8, Figure 5) is then driven to the SEP-1 block where water recovery is simulated and the clean-dry syngas is driven to the next SHIFTING hierarchy. SEP units used in this model are Aspen Plus built-in blocks which separate substances from a mixture by means of mass and energy balances criteria without any thermodynamic equilibrium calculation. In several commercial gasifiers, quenching is used for gas cooling and promotion of slag formation. The water in the WATER-RE stream can be conditioned and reused in the WATQFEED or the WATER inlet streams.

This developed model is useful to predict the syngas composition and reactor temperature under various operating conditions, including flow rates, composition, and temperature of the feed materials as well as the operating reactor pressure.

To simulate the dry feeding technology, the Aspen Plus flow sheet for GASIFIC hierarchy uses just one RGibbs reactor; hence neither mass splitters nor heat splitters are introduced into the model, and the full TO-GASIF stream as well as the full HEAT-1 stream goes to the RGIBB-1 reactor; see Figure 6. Despite this, all the remaining built-in blocks in the dry feeding technology (Figure 6) correspond to the analogous stages that are described in the slurry feeding technology (Figure 5).

3.2.3. SHIFTING Hierarchy. The syngas coming out from GASIFIC hierarchy is sent to the SHIFTING hierarchy, where the WGSR is simulated. As shown in Figure 7, the bypass is simulated by means of a built-in stream splitter block (SPLIT-2). The stream S-9, in the slurry feeding technology, carries between 60% and 70% of SYNGAS stream to the REQUIL reactor. In this reactor, the water gas shift reaction (see (4)) takes place. The stream S-11 leaving the WGSR reactor and stream S-10 (bypass) are mixed and cooled in the HEATER-2 built-in block. The mass flow of the inlet stream STEAM is adjusted until a molar ratio $H_2/CO = 3$ in the stream ADJ-SYNG. To adjust this ratio, the sensitivity analysis tool supported by Aspen Plus was used. This tool is in the section model analysis. The stream ADJ-SYNG leaves the SHIFTING hierarchy and feeds the AGR hierarchy, where gas cleaning process is simulated.

A similar flow sheet presented in Figure 7 is used to simulate the water gas shift process of the dry feeding technology. The process takes into account that through stream S-9 flows around the 85%–95% of SYNGAS stream, while the remaining mass flow bypasses the WGSR reactor through stream S-10.

3.2.4. AGR Hierarchy. In this model, the acid gases recovery unit is modeled by means of a built-in SEP block (SEP-2). The clean-up process is simulated for the syngas by retiring all acid gases and other impurities formed upstream in the process, Figure 8. This stage is similar to both technologies simulated (dry and slurry).

As shown in Figure 8, the ADJ-SYNG stream coming from SHIFTING hierarchy is separated into ACID-G stream (composed by H_2O, N_2, H_2S, NH_3, CO_2, and COS) and TO-METHA stream, which is composed mainly by CH_4, CO and H_2. The stream TO-METHA feeds the next hierarchy where methanation reaction is simulated.

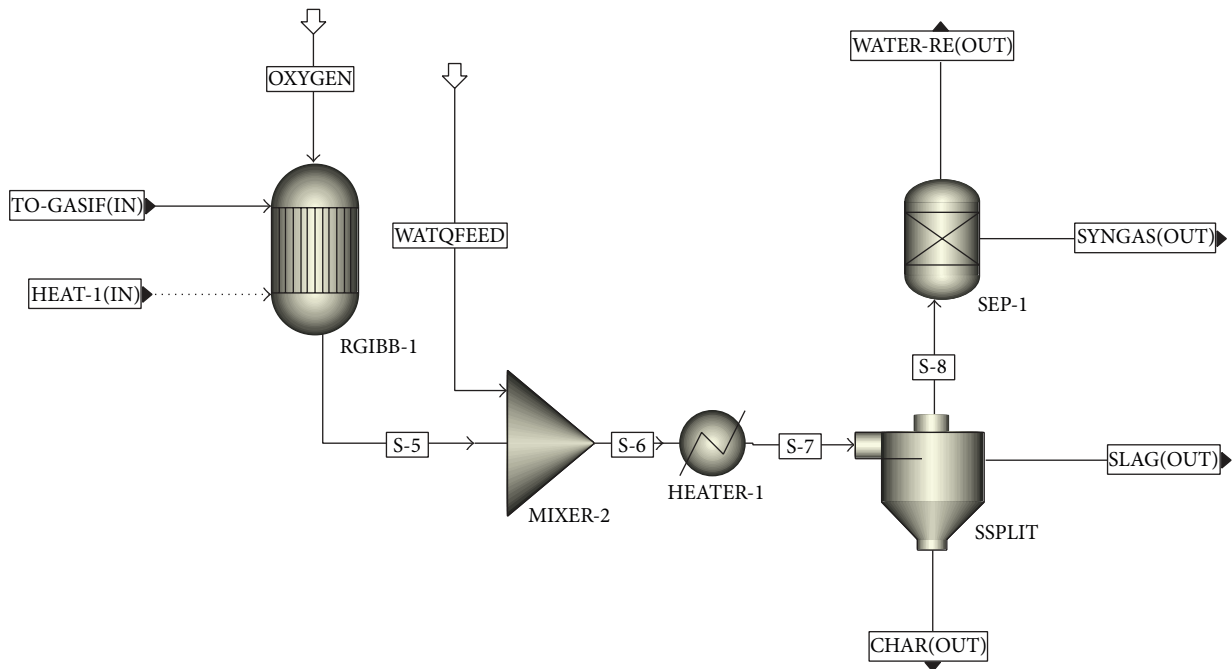*3.2.5. METHANAT Hierarchy.* The stream TO-METHA upcoming from the AGR hierarchy is driven to

FIGURE 6: Aspen Plus GASIFIC hierachy diagram to simulate the gasification stage of coal-GNS process. Flow sheet for dry feeding technology.
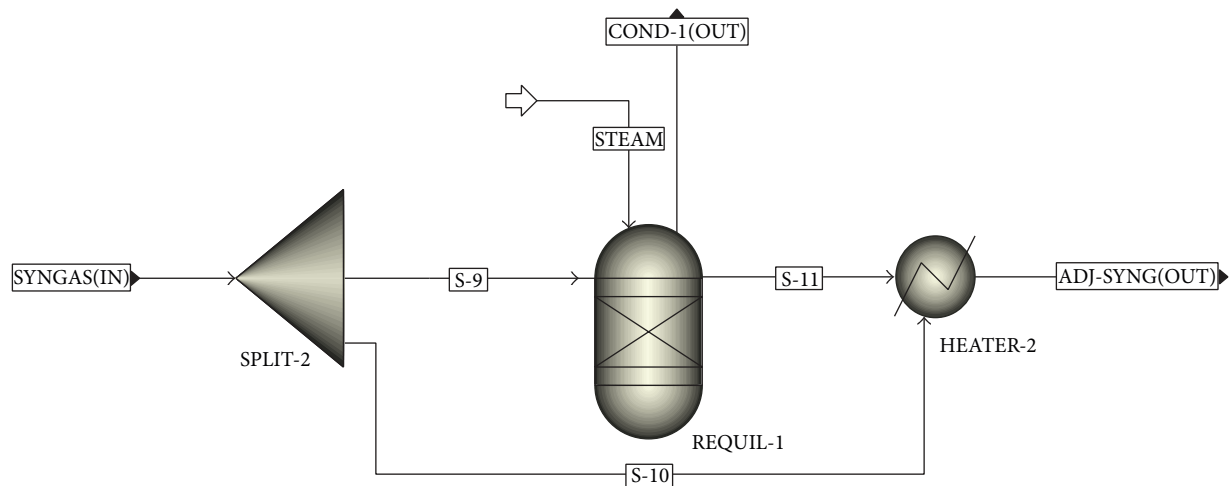

FIGURE 7: Aspen Plus SHIFTING hierachy diagram to simulate the WGSR stage in the coal-SNG process.

the METHANAT hierarchy, where promotion of methane formation is simulated. As shown in Figure 9, the stream TO-METHAN is fed into an equilibrium reactor (REQUIL-2), where CO and H_2 react to form CH_4 and H_2O (see (5)). Condensates are retired by stream S-14, while gaseous products are driven by stream S-12 into a heater (HEATER-3) where the gases are cooled and sent to SEP unit (SEP-3). In the SEP-3 separator, the split process between SNG and water is simulated. CO_2 and any other possible remaining impurities are retired by stream S-15. In this way, the stream SNG (Figure 9) contains the desired gaseous product with high methane concentration.

In this hierarchy, there are no model process differences between the slurry feeding and the dry feeding technology; thus, the dry feeding technology is simulated using the same diagram model (Figure 9).

3.3. Energy Parameters. Energy indicators were estimated to characterize the SNG production via coal gasification using Colombian coals as raw material. These parameters are useful to analyze the process in function of the feeding fuel system technology. The description of such energy indicators is given below.
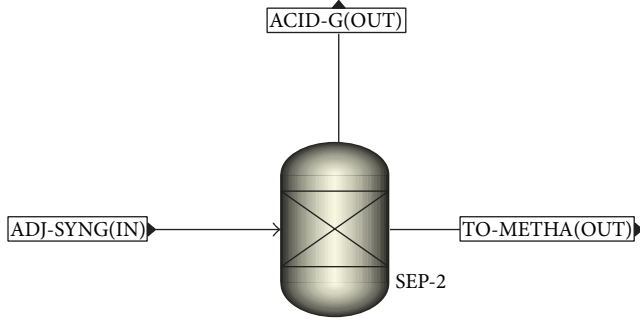
FIGURE 8: Aspen Plus AGR hierarchy diagram to simulate the acid gases clean-up in the coal-SNG process.

TABLE 2: High heating values of the gaseous species considered in the syngas leaving from the gasifier [50].

Gaseous specie	HHV (MJ/Nm^3)	HHV (MJ/kg)
CO	12.622	10.1
H_2	12.769	141.8
CH_4	39.781	55.53
C_2H_4	63	50.2952
C_6H_6	142.893	41.8
H_2S	25.105	16.488
NH_3	13.072	22.428

(i) Equivalence ratio (ER), (7), accounts for the oxygen/coal ratio in the thermochemical process. ER > 1 represents a poor-fuel process while ER < 1 indicates a rich-fuel process or incomplete combustion. ER = 1 indicates stoichiometric combustion, where all the fuel in the gasifier is completely oxidized and transformed into H_2O and CO_2. Consider

$$ER = \frac{\left(\dot{m}_{O_2}/\dot{m}_{coal}\right)}{ER_{stq}}, \quad (7)$$

where $\dot{m}_{O_2}$ and $\dot{m}_{coal}$ are the inlet mass flows of oxygen and coal, respectively. ER_{stq} is the stoichiometric equivalent ratio (see (8)) calculated with the theoretical combustion reaction (see (9)). Consider

$$ER_{stq} = \frac{\varphi \cdot M_{O_2}}{M_{coal}}, \quad (8)$$

$$C_nH_mO_pN_qS_r + \varphi O_2 \longrightarrow aCO_2 + bH_2O + dN_2 + fSO_2, \quad (9)$$
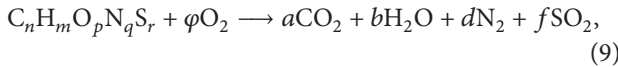
where $C_nH_mO_pN_qS_r$ represents a recursive fuel substitution formula estimated in dry base and ash free; $\varphi = n + m/4 + r/2 - p/2$; M_{O_2} and M_{coal} are the molecular weight of oxygen and coal, respectively.

(ii) Coal Conversion efficiency (CCE, %), (10), is the ratio between the amount (mass units) of SNG at the exit of the process and the amount (mass units) of coal at the inlet of the process. Consider

$$CCE = \frac{\dot{m}_{SNG}}{\dot{m}_{coal}} \times 100 \quad (10)$$

with $\dot{m}_{SNG}$ the mass flow of substitute natural gas leaving the process.

(iii) Cold gas efficiency (η_{cg}, %), or the energy efficiency of the gasification process, (11), is the ratio between the syngas energy in the stream leaving from the gasifier and the coal energy in the stream feeding into the process. Consider

$$\eta_{cg} = \frac{\dot{m}_{syngas} \cdot HHV_{syngas}}{\dot{m}_{coal} \cdot HHV_{coal}} \times 100, \quad (11)$$

where $\dot{m}_{syngas}$ is the mass flow of syngas leaving from the gasifier; HHV_{coal} is the higher heating value of coal as received that is including ash and moisture contents; HHV_{syngas} is the higher heating value of the syngas stream leaving the gasifier (wet basis), (12). Consider

$$HHV_{syngas} = \sum_{i=1}^{k} X_i \cdot HHV_i \quad (12)$$

with X = mass fraction (wet basis); i = each one of the gaseous species with energy contents considered in the syngas, that is, CO, H_2, CH_4, C_2H_4, C_6H_6, H_2S, and NH_3; HHV_i values are taken from the literature and are presented in Table 2 [50].

(iv) Process efficiency (η_{pro}, %), (13), is the energy efficiency of the conversion of the syngas to SNG, estimated as the ratio between energy of SNG on the stream leaving the process and syngas energy on the stream leaving the gasifier, where HHV_{SNG} is the higher heating value of the SNG. Consider

$$\eta_{pro} = \frac{\dot{m}_{SNG} \cdot HHV_{SNG}}{\dot{m}_{syngas} \cdot HHV_{syngas}} \times 100. \quad (13)$$

(v) Global efficiency (η_{global}, %), (14), is defined as the ratio between energy on the SNG stream leaving the process and energy in the coal stream feeding the process, that is, energy efficiency of the coal conversion to SNG. Consider

$$\eta_{global} = \frac{\dot{m}_{SNG} \cdot HHV_{SNG}}{\dot{m}_{coal} \cdot HHV_{coal}} \times 100 = \eta_{cg} \cdot \eta_{pro}. \quad (14)$$

(vi) High heating value of the SNG (HHV_{SNG}), (15), accounts for the quality of the gas leaving the process. It is estimated from the molar fraction of gaseous products with energy content in the SNG stream. Consider

$$HHV_{SNG} = \sum_{j=1}^{n} Y_j \cdot HHV_j \quad (15)$$

with Y = molar fraction; j = each one of the gaseous species with energy content considered in the SNG, that is, CO, H_2, and CH_4.

(vii) Wobbe Index, WI (MJ/Nm^3), (16), accounts for the exchangeability of gases. According to the Wobbe Index, it is possible to know if the SNG quality is good enough to be
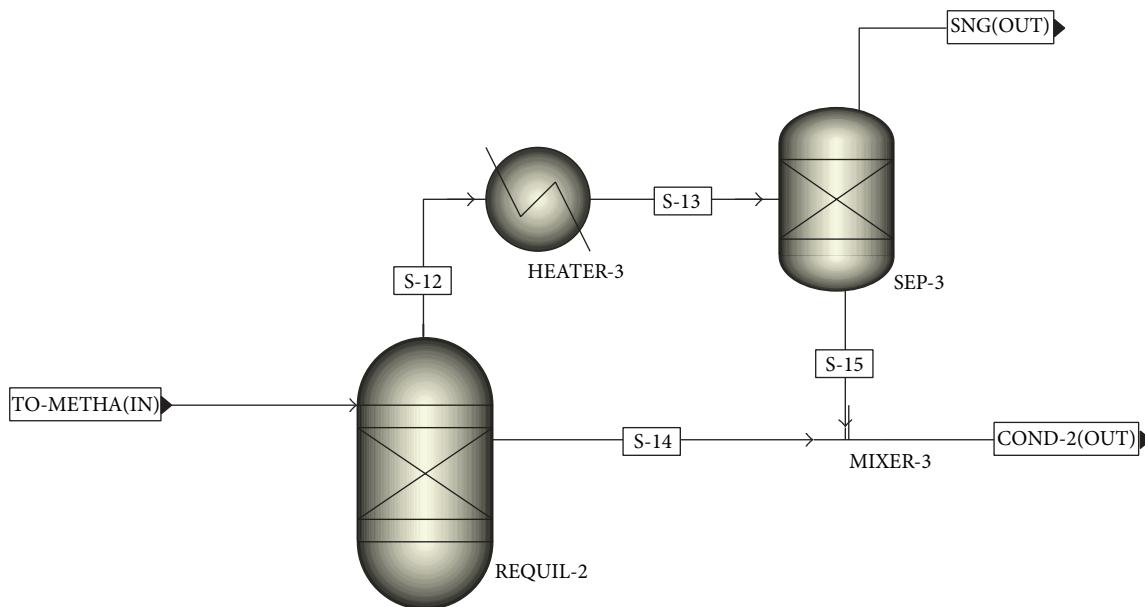
FIGURE 9: Aspen Plus METHANAT hierarchy diagram to simulate the methanation reaction in the cola-SNG process.

transported by gas pipe lines, with density (ρ) at standard conditions (1 atm, 15°C). Consider

$$\text{WI} = \frac{\text{HHV}_{\text{SNG}}}{\sqrt{\rho_{\text{SNG}}/\rho_{\text{air}}}}. \qquad (16)$$

(viii) Power, P (kW), (17), is a parameter referring to SNG power, and it is estimated as the product between SNG mass flow rate produced ($\dot{m}_{\text{SNG}}$, kg/s) and its higher heating value (HHV$_{\text{SNG}}$, kJ/kg). Consider

$$P = \dot{m}_{\text{SNG}} \cdot \text{HHV}_{\text{SNG}}. \qquad (17)$$

3.4. Simulation Conditions. The mass flow rates presented in Table 3 are used to validate the model. The aim is to analyze the model accuracy in order to simulate the SNG production via coal gasification. The operation conditions (i.e., temperature and pressure) for reactors and other facilities (Table 4) were taken from the available technical report [51] or assumed in this work according to the literature or simulation results. The simulation conditions are defined to produce around 100 MMFCD SNG. Therefore, the pressure of the gasifier is higher than 40 bar due to the objective of this work being the study of a real and feasible process [52].

The energy parameters, such as HHV$_{\text{syngas}}$ and HHV$_{\text{SNG}}$, coal conversion efficiency, cold efficiency, process efficiency, global efficiency, Wobbe Index, and power (see (12)–(17)), were directly estimated within the Aspen Plus model by means of Fortran statements in calculator blocks. The equivalence ratio was estimated as an operation condition of the gasifier and thus the reaction temperatures.

4. Results and Discussion

In this section, the simulation results for SNG synthesis with two Colombian coals (Bijao and Sanoha) are compared with available data from the technical report using slurry and dry feeding technologies [51]. Simulation results include the syngas and the SNG compositions, SNG flows (mass and volumetric flows), and energy parameters. These results are useful to compare the feeding technologies as well as fuel specifications (Colombian coal rank) in the SNG production via coal gasification.

Two global parameters to estimate the quality of simulation results and to compare with reference data are proposed in different works, the root mean square deviation (RMSD) or root mean square error (RMSE) and the relative error (RE) [53, 54]. These parameters are considered in this work to analyze the model accuracy against the reference data. The RMSD has the units of each parameter analyzed and the RE is expressed in percentage (%). The RE is presented as the average error between estimated and reported amount of each gaseous specie in the syngas, for both coal types and both feeding technologies. Consider

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{n} \left(X_{\text{reference},i} - X_{\text{model},i} \right)^2}{n}},$$

$$\text{RE} = \left| \frac{X_{\text{reference},i} - X_{\text{model},i}}{X_{\text{reference},i}} \right| \cdot 100. \qquad (18)$$

4.1. Syngas and SNG Composition. The simulated syngas composition for both feeding technologies is validated by comparison with technical report data and it is shown in Table 5. To estimate the model behavior, the RMSD and the RE are presented in the same table. Both comparative parameters have been estimated for each specie in the gas (syngas and SNG) including the coal type and feeding technology in the same calculus.

The coherent behavior of the model to predict the species with higher concentration in the syngas stream is observed.

TABLE 3: Mass flow rates used in the model as inlet streams.

Technology feeding	Raw material	Coal (ton/h)	Water (ton/h)	Oxygen (ton/h)	CO_2 (ton/h)	Steam (ton/h)
Slurry	Bijao	293.6	126.3	173.9	—	86.7*
	Sanoha	219.5	107.1	138.02	—	105*
Dry	Bijao	237.2	—	175.2	143.5	189*
	Sanoha	220.4	—	188	138.2	192.7*

*Estimated in this work, using sensitivity analysis, to reach the ratio $H_2/CO = 3$.

TABLE 4: Reactors temperature and pressure conditions, inlet streams, and other model facilities described in the Aspen Plus models.

Facility or inlet stream	Temperature (°C)	Pressure (bar)
Coal stream	27	1
Water stream	40	5
Oxygen stream	40	74.1
CO_2 stream	100	83
Steam stream	250*	49*
Reactor RGIBB-1 (Figure 5)	Bijao coal: 1658** Sanoha coal: 1413**	50
Reactor RGIBB-2 (Figure 5)	Bijao coal: 940** Sanoha coal: 922**	50
Reactor RGIBB-1 (Figure 6)	Bijao coal: 1340** Sanoha coal: 1508**	50
Reactor REQUIL-1 (Figure 7)	250* (Bijao and Sanoha coals)	49*
Reactor REQUIL-2 (Figure 9)	350* (Bijao and Sanoha coals)	42*
Heater HEATER-1 (Figure 5)	202	Isobaric
Heater HEATER-1 (Figure 6)	167	Isobaric
Heater HEATER-2 (Figure 7)	40	Isobaric
Heater HEATER-3 (Figure 9)	54.7	Isobaric

*Adapted from [25]. **Simulation results.

The RE of H_2, CO, and CO_2 between simulated and reference data varies from 6.6% to 18%. This is confirmed in Table 5 by the lower RMSD of the volumetric concentration of these gaseous species. For example, the RMSD of H_2 indicates that the model prediction varies ±5.3%vol; this value is lower compared with the H_2 concentration produced in the entrained flow gasifiers simulated. The RMSD of CO and CO_2 behaves in a similar way. Nevertheless, the model cannot predict with accuracy the species with lower concentration (traces of N_2, CH_4, NH_3, and COS) in the syngas due to their higher RE. This is also corroborated with the RMSD showed in Table 5. The model variability is higher against the traces concentrations reached in the gasification technologies simulated.

It is important to highlight that the temperature operation of the gasifier was not available in the reference work and thus could be an important deviation source between the reference and simulated data.

Regarding the HHV_{syngas} (wet basis), a fundamental energy parameter to characterize the gasification process, it is highlighted that the model is able to predict coherently this factor, because its RE is 13% and its RMSD varies in ±1.6 MJ/Nm³. The higher heating value is around 10 MJ/Nm³ for both raw materials and both technologies simulated. These results are quite similar to other coal gasification reports that use the chemical equilibrium approach for their simulations [24].

Despite the low accuracy of the model to estimate traces but considering the HHV_{syngas} as global parameter of the process, it is possible to state that the gasification model behaved coherently under different coal types and feedstock feeding technologies.

Table 6 compares the composition of SNG between simulated conditions in this work and reported data [51]. Table 7 shows the mass and volumetric flows of SNG produced as well as the HHV_{SNG} (see (15)), Wobbe Index (see (16)), and power (see (17)).

Methane concentrations in the simulated SNG are comparable for both technologies (Table 6) independent of coal type. The average RMSD of SNG composition is ±1.8%vol and the average relative error between reported and simulated data is lower than 2%. However, the yield of CH_4 with slurry feeding technology tends to be slightly higher due to the two gasification stages. Methane composition in the SNG simulated for both technologies is closer to Colombian natural gas composition from the *Guajira* region (around 97%vol of CH_4).

On the other hand, in all simulated cases the model is not able to predict the traces concentration of H_2, N_2, and CO_2 in the SNG stream. The RE of simulated data for

TABLE 5: Validation of syngas composition (vol% dry base) for two different Colombian coals under slurry and dry feeding technologies.

Syngas ($\%vol_{d.b.}$)	Slurry feeding				Dry feeding				RMSD (units)	$\overline{RE}^*$ (%)
	Bijao		Sanoha		Bijao		Sanoha			
	[51]	Model	[51]	Model	[51]	Model	[51]	Model		
N_2	0.61	0.35	0.6	0.3	1.27	0.628	1.26	0.61	3.6	48.7
H_2	37.10	35.39	30.9	38.52	26.06	20.58	26.25	20.19	5.3	18.3
CO	37.88	37.07	44.9	42.27	64.49	69.45	65.29	72.41	3.3	6.6
CO_2	20.64	22.08	14.0	13.98	7.6	8.80	6.61	6.26	1.5	7.1
CH_4	3.24	3.89	9.0	3.74	0.01	0.02	0.01	0.01	2.7	44.6
H_2S	0.44	0.44	0.5	0.42	0.42	0.41	0.42	0.41	0.8	5.2
NH_3	0.01	0.7	0.0	0.71	0.03	0.002	0.03	0.00	5.0	2364.4
COS	0.02	0.02	0.0	0.02	0.03	0.06	0.03	0.07	5.8	77.8
Ar	0.04	0.05	0.0	0.04	0.05	0.04	0.06	0.05	2.0	20.6
$HHV_{w.b.}$ (MJ/Nm^3)	8.49	7.44	11.77	9.06	9.28	10.66	11.47	11.1	1.6	13.4

*Calculated as the average of the four pairs simulation-reported data described in each entire row.

TABLE 6: Comparison between SNG compositions simulated and reported data under slurry and dry feeding technologies.

SNG (% vol.)	Slurry feeding				Dry feeding				RMSD (units)
	Bijao		Sanoha		Bijao		Sanoha		
	[51]	Model	[51]	Model	[51]	Model	[51]	Model	
H_2	0.33	1.17	0.32	1.07	0.31	1.11	0.31	1.22	0.8
CH_4	97.83	95.98	98.2	96.55	94.11	96.02	94.18	96.05	1.8
CO_2	0.07	0.00	0.07	0.00	0.06	0	0.06	0.00	0.1
N_2	1.55	2.68	1.23	2.25	5.3	2.69	5.19	2.54	2.0
Ar	0.23	0.17	0.17	0.13	0.21	0.18	0.26	0.19	0.1

these species compared with the reference data is higher than 65%. This can be seen in Table 6, where the RMSD of the traces is higher compared with the concentration produced in the gasification process. However, it is important to highlight the relative small magnitude order for H_2, Ar, N_2, and CO_2 concentration levels (lower than 2%vol) against to the CH_4 concentration in the SNG (between 94 and 98%vol). Therefore, the traces concentration has a negligible effect on the energy parameters estimated in Section 4.2.

4.2. SNG Production and Quality As Gaseous Fuel. Despite the model low accuracy to predict the traces in the SNG stream, in Table 7, it can be observed that HHV_{SNG} calculated by the simulations is almost equal for both Sanoja and Bijao Colombian coals (independent of the feeding technology), and in both cases HHV_{SNG} is quite similar to the reported data in the literature. The average relative error of HHV_{SNG} is lower than 2%; this can be explained due to similar CH_4 contents (Table 6) obtained from methanation stage. Thereby, feeding technology would not affect HHV_{SNG}. According to HHV_{SNG} and WI_{SNG} presented in Table 7, the simulated SNG can be classified as a high quality natural gas (NG) and it can be transported by gas pipe lines (for both coals and both technologies used) [22]. The high quality classification is due to the fact blank that HHV_{SNG} and WI_{SNG} parameters are between the ranges defined by Colombian regulatory

norms. HHV_{NG} must be between 35.4 and 42.8 MJ/m^3 and WI 47.7–52.7 MJ/m^3 [55]. Therefore, the SNG produced and distributed can be used in transport, power, and heat generation in industrial and domestic systems [21]. Thereby, the SNG can contribute to meet the increasingly high demand of the gaseous fuel in Colombia.

It is evidenced in Table 7 that for both feeding technologies the simulation of SNG production from Colombian coal gasification does not show significant differences (in mass flows or volumetric flows) when compared with reference report [51]. This is due to the coherent RE that varies between 2.7% and 4.2%. Therefore, the models developed in this work can be considered as computational tools to study the coal to SNG process. The differences between simulated and reference data can be attributed to the unavailability of STEAM flow rates in the reported data (Table 4) and its incidence in global mass balances.

Regarding the power of the SNG (Table 7), the values calculated are between the expected error boundaries due to mass flow and HHV differences among simulations and reported data. The power is overestimated by 9.5% with both coals without relying on the technology. The higher potential energy obtained for Sanoha coal is due to its better quality as fuel (Table 1).

4.3. Mass and Energy Efficiencies. The carbon conversion efficiency (CCE) is presented in Figure 10. It is observed that

TABLE 7: Model validation with regard to SNG production and quality as gaseous fuel.

Energy parameter	Slurry feeding				Dry feeding				RMSD (units)	$\overline{RE}^*$ (%)
	Bijao		Sanoha		Bijao		Sanoha			
	[51]	Model	[51]	Model	[51]	Model	[51]	Model		
HHV_{SNG} (MJ/Nm^3)	39	38.33	39.1	38.55	37.5	38.34	37.5	38.37	0.74	1.9
Mass flow (kg/h)	78400	81006	82700	86063	79300	80504.8	82000	80332	2362.98	2.7
Volumetric flow (MMFCD)	96.81	101.18	102.51	107.49	95.3	100.55	98.56	100.34	4.32	4.2
WI (MJ/m^3)	51.6	51.68	51.9	51.98	49	51.70	49	51.73	1.92	2.8
Power (MW)	1147	1250	1221	1328	1107	1242	1146	1239	110.6	9.5

*Calculated as the average of the four pairs simulation-reported data described in each entire row.
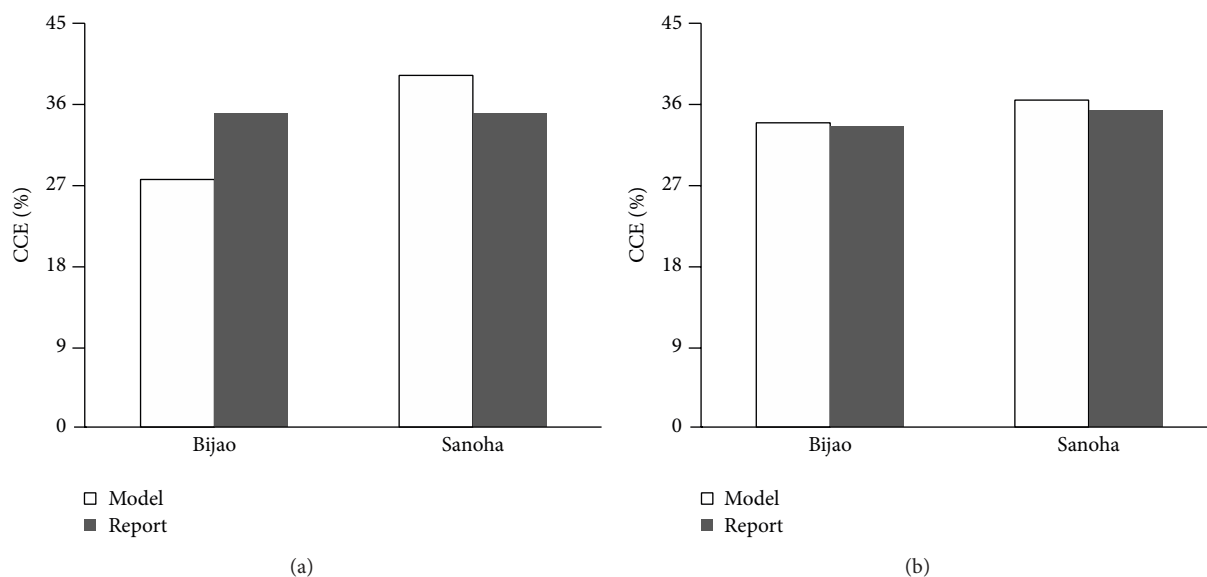

FIGURE 10: Carbon conversion efficiency (kg CH$_4$/kg coal). Comparison for simulated and reported data for two Colombian coals; (a) slurry feeding technology and (b) dry feeding technology.

Sanoha coal tends to give higher coal conversion, especially with the slurry feeding technology. This could be explained by the higher volatile matter contents of this coal (Table 1); and because of the slurry feeding technology, the first one of two gasification stages operates at higher temperatures than the gasifier dry feeding technology (Table 4).

The difference between simulated CCE and technical report data is about 3.5%. Moreover, the simulated data agree with biomass gasification yields reported in the literature, around 26% kg CH$_4$/kg wood [25]. Differences of CCE around 3%-4% between coal and wood as raw material can be explained by the coal higher fixed carbon with regards to wood or biomass.

It is observed from Figure 11 that cold gas efficiency is slightly higher for dry feeding technology, as expected according to the literature [12]. This trend is due to the slurry feeding technology requiring more energy for the autothermal process to vaporize water in the gasifier. Nevertheless, relative differences between reported and simulated data are almost meaningless, independent of the coal or the simulated technology.

Figure 12 shows that process efficiency is higher for the slurry feeding technology when compared with dry feeding technology, independent of the coal. This is explained because the higher methane content in syngas from slurry technology produces a higher syngas quality to be fed into the catalytic methane reactor. The same trend is observed in the comparison of global efficiencies, Figure 13.

From Figures 10–13, it can be observed that even when efficiencies estimated by the simulations with dry technology are slightly lower than those obtained with slurry feeding technology, the average margin of error between the model and technical report is less than 5%. It is clear that the process efficiency (Figure 12) is 3% higher for Sanoha coal with regard to Bijao coal. This is due to the Sanoha coal having a higher quality rank than Bijao coal (Table 1).

The process and global efficiencies are higher for slurry feeding technology (Figures 12 and 13). This is due to the higher hydrogen concentration in the syngas produced with the slurry feed technology against dry feed technology [21].

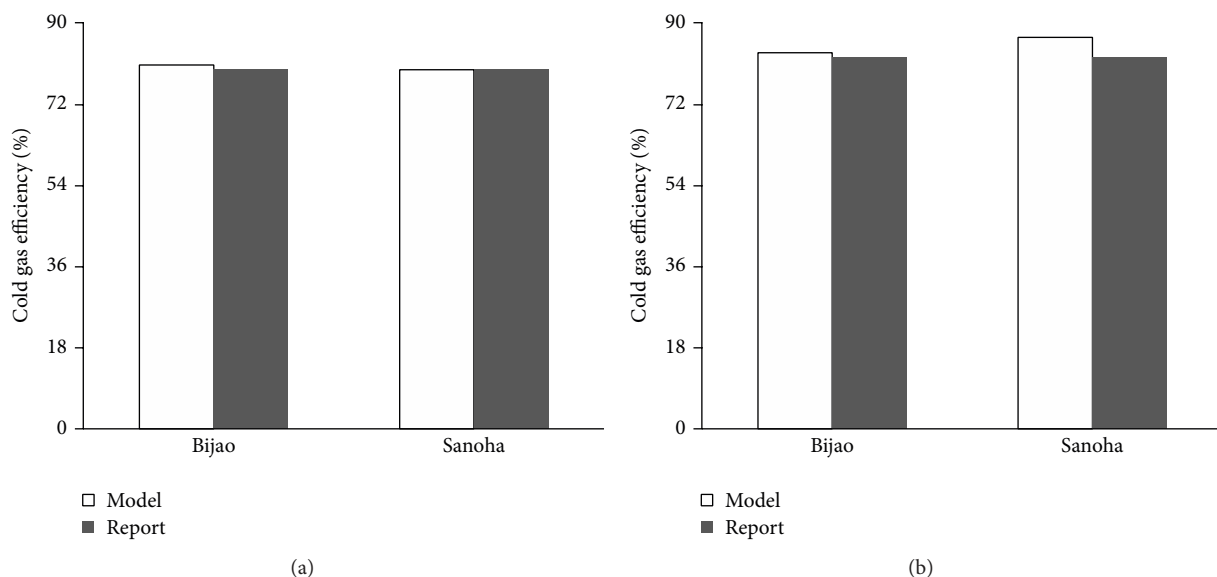The slurry feeding technology tends to be more efficient than dry feeding technology in the process of coal to SNG

FIGURE 11: Cold gas efficiency (%). Comparison between simulated and reported data for two Colombian coals; (a) slurry feeding technology and (b) dry feeding technology.
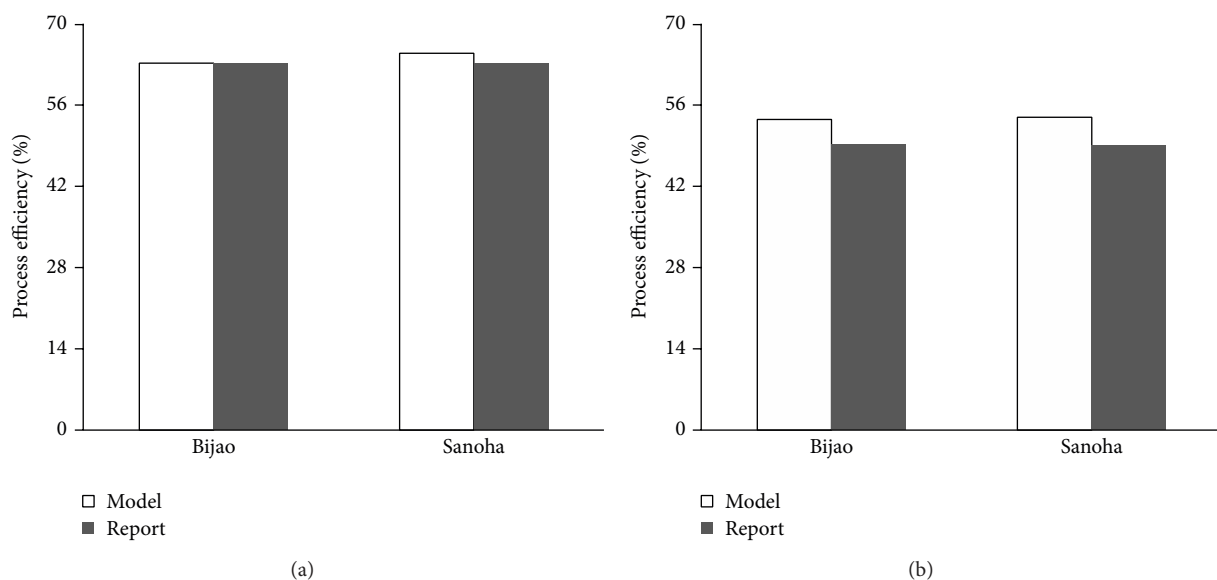

FIGURE 12: Process efficiency (%). Comparison between simulated and reported data for two Colombian coals; (a) slurry feeding technology and (b) dry feeding technology.

simulated in this work. Differences in these parameters were not found in function of the coal rank. The cold gas efficiency is similar to all simulated cases with a slightly improvement for dry feeding technology. The gasification efficiency is better for Sanoha coal due to its fixed carbon content and higher HHV_{coal} (Tables 1 and 5).

The RMSD was estimated accounting all data presented. Low differences between simulated and reported data, for both coals using the two different feeding technologies, were found. These values indicate a good agreement between simulated data with the models described in this study and reported data available from the literature. Therefore, the model developed in this paper constitutes a valuable and versatile tool to study the thermodynamic performance of the solid fuels to SNG process via gasification.

5. Conclusions

A model to simulate the SNG production via coal gasification process has been developed using Aspen Plus software. The model considers two different typical technologies to supply the fuel into the gasification process. The feeding systems are coal-water slurry and dry coal. The model can simulate different solid fuel types. Therefore, the effect of using two different Colombian coals, Bijao and Sanoha, is considered in this work.
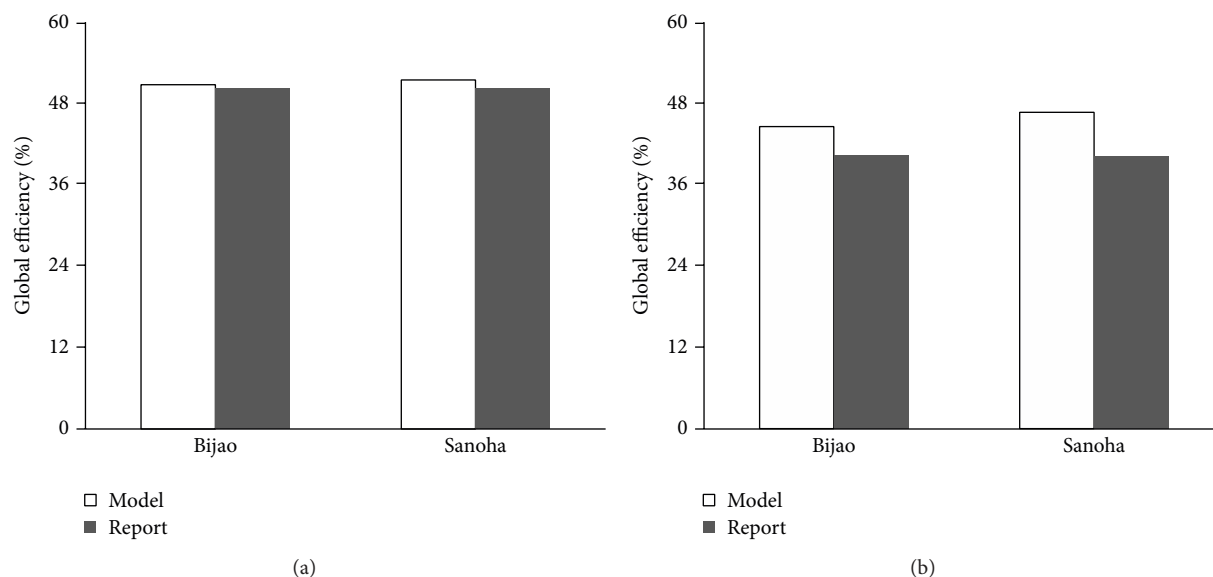
FIGURE 13: Global efficiency (%). Comparison between simulated and reported data for two Colombian coals; (a) slurry feeding technology and (b) dry feeding technology.

A global comparison between reported and simulated data presents an average relative error lower than 13%. Therefore, the developed model is able to predict the composition and heating values of syngas and SNG and the SNG quality and energy parameters of the process and the trends. The computational model presented in this work and developed in Aspen Plus v7.3 software can be used for gaining a fundamental understanding of the engineering and optimization of the process, even when scaled up.

According to the simulation process, it was found that coal rank does not significantly affect energy indicators such as cold gas, process, and global efficiencies. However, feeding technology clearly has an effect on these energy parameters. The process and global efficiencies are higher for slurry feeding technology, while cold gas efficiency was higher for dry feeding technology; these results agree with the literature. According to HHV_{SNG} and WI, the simulated SNG from both coals and both technologies can be classified as a high quality NG in Colombia. Therefore, the gaseous fuel can be transported by gas pipe lines and the SNG can contribute to meet the increasingly high demand of the gaseous fuel in Colombia.

Since the proposed model can be used to analyze various types of entrained flow reactors with different operating conditions, it can be considered a versatile and useful computational tool to optimize the coal to SNG process. In a future work, a sensitivity analysis of the effect of Colombian coal rank (subbituminous to semi-anthracite) will be conducted.

Nomenclature

AGR:	Acid gas recovery unit
CCE:	Coal conversion efficiency (%)
CGE:	Cold gas efficiency (%)
d.b.:	Dry basis
ER:	Equivalent ratio (-)
ER_{stq}:	Stoichiometric equivalence ratio (-)
HHV:	Higher heating value (kJ/Nm^3)
IGCC:	Integrated gasification combined cycle plant
$\dot{m}$:	Mass flow (kg/s)
M:	Molecular weight (kg/kmol)
MMFCD:	Millions of cubic feet per day
n, m, p, q, r:	Molecular subindex of recursive fuel substitute formula
P:	Thermal power of synthetic natural gas (kW)
RE:	Relative error
$\overline{RE}$:	Average relative error
RMSD:	Root mean squared deviation (-)
R/P:	Reserves-to-production ratio
SNG:	Synthetic or substitute natural gas
USW:	Urban solid wastes
w.b.:	Wet basis
WGSR:	Water gas shift reactor
X_i:	Mass fraction of substance i (-)
Y_j:	Molar fraction of substance j (-)
WI:	Wobbe Index (MJ/Nm^3)
η_{cg}:	Cold gas efficiency (%)
η_{global}:	Global efficiency (%)
η_{pro}:	Process efficiency (%)
φ:	Hypothetical stoichiometric coefficient (mol)
ρ:	Density (kg/m^3).

Aspen Plus Model Hierarchy Acronyms

AGR:	Hierarchy for acid gas recovery unit
FEEDING:	Hierarchy for slurry preparation

GASIFIC: Hierarchy for gasification stage
METHANAT: Hierarchy for methanation stage
SHIFTING: Hierarchy for water gas shift reactor.

Aspen Plus Model Built-In Blocks Acronyms

HEATER-1, HEATER-2, and HEATER-3:	Heater units
MIXER-1, MIXER-2, and MIXER-3:	Mixer units
REQUIL-1, REQUIL-2:	Equilibrium reactor units
RGIBB-1, RGIBB-2:	Gibbs reactor units
RYIELD:	Yield reactor unit
SPLIT1, SPLIT-2, QSPLIT, SSPLIT, SEP-1, SEP-2, and SEP-3:	Separation units or stream divisor units.

Aspen Plus Model Streams Acronyms

ACID-G, ADJ-SYNG, CHAR, CO2, COAL, COND-1, COND-2, H-2, H-3, HEAT-1, OXYGEN, S-1, S-2, S-3, S-4, S-5, S-6, S-7, S-8, S-9, S-10, S-11, S-12, S-13, S-14, S-15, SLAG, SNG, STEAM, SYNGAS, TO-GASIF, TO-METHA, WATER, WATER-RE, WATQFEED.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgment

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