Dynamic modelling and simulation of IGCC process with Texaco gasifier using different coal

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Integrated gasification combined cycle (IGCC) is considered as a viable option for low emission power generation and carbon dioxide sequestration. As a part of the process of IGCC plant design and development, modelling and simulation study of the whole IGCC process is important for thermodynamic performance evaluation, study of carbon capture readiness and economic analysis. The work presented in the paper is to develop such a whole system model and simulation platform. A simplified dynamic model for the IGCC process is developed, in which Texaco gasifier is chosen to give the basic representation for the IGCC process. The chemical equilibriums principle is used to predict the syngas contents in the modelling procedure. The influences of key parameters to regulate the input such as oxygen/coal ratio and water/coal ratio to syngas generation are studied. The simulation results are validated by comparing with the industry data provided by the Lu-nan fertilizer factory. Water-shift reactor, gas turbine and heat recovery steam-generation modules are modelled to study the dynamic performance with respect to the variation from the input of syngas stream. The simulation results reveal the dynamic changes in the plant outputs, including gas temperature, power output and mole percentages of hydrogen and carbon dioxide in the syngas. The process dynamic responses with three types of coal inputs are studied in the paper and their dynamic variation trends are presented via the simulation results.

Keywords: chemical equilibrium; dynamic performance; IGCC; syngas; Texaco gasifier

Nomenclature

- $A$: carbon conversion rate
- $C_p$: specific heat capacity
- $N$: molar flow rate
- $D$: derivative
- $H$: enthalpy
- $\Delta H_f$: enthalpy of formation
- $T$: Kelvin temperature
- $X$: mole fraction
- $S$: simulation
- $R$: reference
- $P$: pressure
- $Ar$: Argon
- $C$: carbon
- $CH_4$: methane
- $CO$: carbon monoxide
- $CO_2$: carbon dioxide
- $COS$: cabonyl sulphide
- $H$: hydrogen
- $H_2$: hydrogen element
- $H_2O$: water, vapour
- $H_2S$: hydrogen sulphide

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merits for integration with carbon capture and storage units. Figure 1 shows a schematic diagram of the whole IGCC process which is, no doubt, a complicated energy conversion process formed by many interconnected subsystem modules. In the IGCC process, the coal slurry and oxygen react in the gasifier and generate syngas primarily made of H₂ and CO. The WGS raises the H₂ and CO₂ concentration while reducing the CO content. The sweet syngas combustion in the gas turbine will generate power and hot flue gas, which is used in HRSG to generate power as well.

The work on IGCC process modelling can be dated back to the 1970s. Researchers in the chemical engineering field studied the coal gasification process and developed models based on mass and energy balances (Beér, 2000; Brown, Smoot, & Hedman, 1986; Buskies, 1996; Chen et al., 2004; Govind & Shah, 1984; Ni & Williams, 1995; Smoot & Smith, 1979; Ubhayakar, Stickler, & Gannon, 1977;Watkinson, Lucas, & Lim, 1991; Wen & Chaung, 1979). Researchers in thermal engineering developed gas turbine and steam power plant models (Colonna & van Putten, 2007; Lu & Hogg, 2000; van Putten & Colonna, 2007). However, dynamic modelling of the whole process is still not mature and requires further study.

Among all the sub-modules of the IGCC process, the most important and complicated one is the one for the gasifier. The challenge of modelling the gasification process will need to deal with complicated chemical reactions involved in the process. The earliest report on modelling this process was published in the 1970s (Ubhayakar et al., 1977), in which a one-dimensional model was reported with consideration of fluid mix in the axial direction. Smoot and Smith (1979) provided an approach to evaluate different chemical kinetics data and to estimate the input parameters; this method has laid the foundation of many subsequent works. Wen and Chung (1979) built a model of Texaco gasifier which divided the furnace into three zones to describe the processes from pyrolytic cracking to gasification; mass balance and energy balance equations are built for each zone. Govind and Shah (1984) introduced momentum conservation to the former work and calculated the temperature, concentration and fluid field in the axial direction.

Most of the models reported in the published literature are based on experimental data using a data-driven approach, which limits the suitability of a model for industry use as its working conditions vary in a wide range. To provide good prediction for syngas output, a generic gasifier model is developed based on the process engineering operation principles discussed in this paper and its steady-state prediction is validated. The syngas output stream from the gasifier varies depending on the reactions in the gasifier and the coal slurry feeding speed. It increases from its initial rate of 0.1 mol/s to settle at 100 mol/s in 100 s.

The auxiliary modules including shift reactor, gas turbine, and HRSG are built with Matlab and a Simulink-based toolbox – Thermolib. The syngas generated by the gasifier will first enter a water quencher and will then be further cooled by a syngas cooler. After hydrolysis reaction and desulphuration reaction, the COS and H₂S contents in the syngas will be removed. The sweet syngas will then pass the shift reactor where the CO contents will be shifted to hydrogen and CO₂, which not only can enhance the fuel gas quality but also raise the CO₂ concentration. After the shift reaction, the shifted syngas will be compressed and heated again and injected to the gas turbine to generate electricity; the heat carried by the exhaust gas will be utilized to generate superheated steam in HRSG and

Figure 1. Simplified schematic diagram of an IGCC system (Casella & Colonna, 2012).
produce more electricity, thus improving the overall system efficiency.

2. Description of Texaco gasifier and mathematical model

Texaco gasification technology, also known as coal slurry gasification technology, is developed by Texaco Company, initially for heavy oil gasification applications. Texaco gasifier structure is shown in Figure 2. It gasifies coal slurry, which is mixed by pulverized coal particles and water, as raw material, and uses oxygen as the gasification agent. Coal slurry is injected into the gasifier furnace through nozzles; the moisture content of coal slurry droplets will evaporate rapidly and the pulverized coal particles will devolatilize and yield coal tar, gaseous hydrocarbons and oil. The gaseous components and volatiles will be consumed rapidly with steam and oxygen. The combustion of carbon char will react with oxygen, carbon dioxide and hydrogen while the reaction products react with each other as well. The whole gasification process involves complicated physical and chemical reactions. The gasifier generates wet syngas composed of CO, CO₂, H₂ and steam. Syngas will leave the gasification zone with slag and enter the water quench zone where the slag will be deposited in the slag tank. Raw syngas will be cooled and cleaned after the quenching process.

The mathematic model for this process is developed by following the work of Watkinson et al. (1991). To simplify the modelling procedure, the following assumptions are made:

1. The flow in the gasifier furnace is uniformed laminar flow, and the differences in temperature, concentration, pressure and material exchanges in the radial direction are not taken into consideration. Actually, laminar flow only exists in the lower part of the gasifier; the flow between nozzles and the lower part should be jet flow surrounded by a strong back flow zone. The eddy turbulent is not considered in the modelling process as the syngas content will not be affected by this flow type. Thus, it is acceptable for the global laminar assumption.

2. Preheating of slurry droplets, moisture evaporation and coal devolatilization will be complete as soon as the coal slurry is injected into the gasifier. The nozzles are surrounded by high-pressure high-temperature gas flow.

3. The released volatile combustion and carbon pyrolytic and char combustion reactions reach chemical equilibrium as soon as the slurry enters the furnace. The chemical equilibrium constants of homogeneous reactions inside the gasifier are used to describe the reactions.

4. Nitrogen and argon are assumed to be steady and will not participate in any chemical reaction. It is assumed that all oxygen is consumed, and the carbon conversion is 99.5% in the entire gasifier.

Chemical reactions considered in this paper are as follows:

\[
\begin{align*}
C + O_2 & \rightarrow CO_2, \\
C + \frac{1}{2}O_2 & \rightarrow CO, \\
C + H_2O & \rightleftharpoons H_2 + CO, \\
C + CO_2 & \rightleftharpoons 2CO, \\
CO + H_2O & \rightleftharpoons H_2 + CO_2, \\
CO + 3H_2 & \rightleftharpoons CH_4 + H_2O, \\
SO_2 + 3H_2 & \rightleftharpoons H_2S + 2H_2O, \\
COS + H_2O & \rightleftharpoons H_2S + CO_2.
\end{align*}
\]

For the aforementioned chemical reactions, mass balance equations of carbon, oxygen, hydrogen, nitrogen and sulphur can be derived as follows:

\[
\begin{align*}
N_{C,0}A &= N_g(X_{CO} + X_{CO_2} + X_{CH} + X_{COS}), \\
N_{O_2,0} &= N_g(0.5X_{CO} + X_{CO_2} + X_{SO_2} + 0.5X_{COS} \\
&\quad + 0.5X_{H_2O}), \\
N_{H_2,0} &= N_g(2X_{CH_4} + X_{H_2S} + X_{H_2} + X_{H_2O}).
\end{align*}
\]
\[ N_{N_2,0} = N_g(X_{N_2}), \]  
\[ N_{S,0} = N_g(X_{SO_2} + X_{H_2S} + X_{CO}), \]  
\[ N_{Ar,0} = N_g(X_{Ar}). \]

According to Dalton’s law (Watkinson et al., 1991), we have

\[ X_{CO} + X_{CO_2} + X_{CH_4} + X_{H_2} + X_{H_2O} + X_{H_2S} + X_{SO_2} + X_{CO} + X_{N_2} + X_{Ar} = 1. \]  
(15)

Equations (9)–(14) are derived based on the mass conservation of C, O, H, N, S and Ar. From Dalton’s law (Watkinson et al., 1991), Equation (15) means that the sum of all the syngas contents equals 1.

Based on chemical equilibrium:

\[ \frac{X_{H_2}X_{CO}}{X_{CO}X_{H_2O}} = 0.0265 e^{3056/T_g}, \]  
(16)

\[ \frac{X_{CH_4}X_{H_2O}}{X_{CO}X_{H_2}P^2} = 6.7125 \times 10^{-14} e^{27020/T_g}, \]  
(17)

\[ \frac{X_{H_2S}X_{H_2O}}{X_{SO_2}X_{H_2}P} = 4.3554 \times 10^{-4} e^{26281/T_g}, \]  
(18)

\[ \frac{X_{H_2S}X_{CO}}{X_{CO}X_{H_2O}P} = 0.75314 e^{4083/T_g}. \]  
(19)

Equations (16)–(19) are derived based on the chemical equilibrium of reactions (5)–(8) listed earlier; the reaction temperature and pressure will affect the equilibrium and change the concentration of syngas contents. There are 11 variables in Equations (9)–(19); this nonlinear equation system can be solved using the Newton–Raphson method (Wang, Wang, Guo, Lv, & Gao, 2013). Energy balance can be expressed as \{Total enthalpy input\} − \{Total enthalpy output\} = \{Heat loss to environment\}; the enthalpy input includes raw material enthalpy, the chemical reaction formation enthalpy and enthalpy carried by recycled gas. The enthalpy output includes enthalpy carried by output syngas, tar and char. Gaseous enthalpies are calculated as

\[ H_{g,i} = N_g \left[ \sum_i X_i \left( \Delta H_{f,i} + \int_{298}^{T_g} C_P(i) dT \right) \right]. \]  
(20)

3. Governing equations

In the Thermolib toolbox, the syngas stream is organized as a vector formed by the data flow of mole flow, contents concentration, temperature, pressure, enthalpy flow, entropy flow, Gibbs energy rate, heat capacity rate and vapour fraction of all compounds, which is described as combined flow bus. The gas phase contents are considered as the real gas form, and their enthalpy, entropy and heat capacity rate will be calculated by using the Peng–Robinson real gas equations of state (Peng & Robinson, 1976).

The most important governing equations are formed of mass balance and energy balance; the mass balance for a normal (standard) block is as follows:

Mass balance:

\[ \frac{dM_i}{dt} = \sum Y_{i,in} M_{in} - \sum Y_{i,out} M_{out} + \sum R_i. \]  
(21)

where \( Y_{i,in} \) denotes the mass concentration of content \( i \) in inlet flow, \( M_{in} \) denotes the inlet mass flow rate, \( Y_{i,out} \) denotes the mass concentration of content \( i \) in outlet flow, \( M_{out} \) denotes the outlet mass flow rate and \( R_i \) denotes the net production rate of \( i \) by chemical reactions.

When no chemical reaction occurs in the simulated block, the factor \( R_i \) will equal zero. In addition, mass accumulation is not considered in all the blocks simulated in this paper.

The governing equation of energy balance is derived by following the first law of thermodynamics:

\[ \frac{dU}{dt} = \sum \dot{H}_{i,in} - \sum \dot{H}_{j,out} + \sum \dot{Q}_k + \sum \dot{P}_m, \]  
(22)

where \( U \) denotes the internal energy in block, \( \dot{H}_{i,in} \) denotes the enthalpy flow rate of content \( i \) in the inlet flow, \( \dot{H}_{j,out} \) denotes the enthalpy flow rate of content \( j \) in the outlet flow, \( \dot{Q}_k \) denotes the heat flow and \( \dot{P}_m \) denotes the mechanical power.

All the auxiliary blocks built with Thermolib in this paper will follow Equations (21) and (22). The individual blocks will be explained one by one in the following.

4. Description of the WGS reactor

The syngas generated by the gasifier will be cooled in the quench water pool. The wet syngas will then enter the WGS and the exothermic water gas shift reaction will take place:

\[ CO + H_2O \rightleftharpoons H_2 + CO_2. \]  
(23)

In the industry, a shift catalyst is used in the reactor; the catalyst can convert most of the CO to \( CO_2 \) with the evolution of heat. There are a number of specific advantages from incorporating a shift reactor into the coal gasification flow scheme in real world; it will improve the \( H_2 \) extraction while decreasing the \( CO \) concentration in the syngas stream. The shift reactor with heat recovery is able to increase the power output for the same gas turbine investment as well. Moreover, the WGS is important for the preparation of \( CO_2 \) sequestration because the \( CO_2 \) concentration rises as well. Moreover, the WGS is important for the preparation of \( CO_2 \) sequestration because the \( CO_2 \) concentration rises as well. Additionally, the WGS is important for the preparation of \( CO_2 \) sequestration because the \( CO_2 \) concentration rises as well. Additionally, the WGS is important for the preparation of \( CO_2 \) sequestration because the \( CO_2 \) concentration rises as well.
be developed and validated for this simulation; thus, a reaction rate-controlled reactor block developed using the Thermolib toolbox is adopted to simulate the WGS reaction process, and the heat exchange with the environment is considered.

In this mode, two shift reactors are connected in series and the reaction rates are defined, respectively, as 0.8 and 0.9 (Karmarkar, 2005); meanwhile, the pressure loss and heat exchange with the environment are considered. By defining the reaction rate, the conversion of CO can be controlled; thus, the partial pressure of CO2 in the shifted syngas will satisfy the demand for further PSA carbon capture simulation. The development of the carbon capture model and its integration with the current IGCC model will be studied in the future.

Based on the energy balance, the reactor model in the WGS process can be described by

$$\sum m_{\text{in}}h_{\text{in}} = \sum m_{\text{out}}h_{\text{out}} + Q.$$  \tag{24}

The syngas temperature, pressure, mass flow rate and contents dynamic change are obtained. In this paper, the contents of the syngas entering the WGS are simplified as a mixture of CO, CO2, H2 and H2O only. This simplification will not cause big error because the total portion of CH4, N2, H2S, SO2, COS and Ar is less than 2% in the syngas, and they will not affect the model to represent the process correctly in terms of the dynamic features concerned in the analysis.

5. Description of the gas turbine

The gas turbine-centred power-generation process is based on Brayton cycle (Lichty, 1967). It has a rotating compressor coupled to the shaft of the turbine, and a combustion chamber in between. The shifted syngas is compressed, mixed with compressed air in the mixer and then ignited in the combustion chamber. The combustion of H2 under a constant pressure will generate the hot flue gas. The flue gas expands through the turbine to perform work.

An isentropic compressor developed in Thermolib is adopted to model the compression process; this block can increase the pressure of an incoming flow to a given outlet pressure. To achieve more accurate simulation results, a certain isentropic efficiency is given in this process modelling, which can decrease the error between simulation results and practical working conditions. The isentropic efficiency is defined by Equation (25):

$$\eta_s = \frac{h_{\text{out},s} - h_{\text{in}}}{h_{\text{out}} - h_{\text{in}}},$$ \tag{25}

where $h_{\text{out},s}$ is the enthalpy in ideal isentropic state, while $h_{\text{out}}$ is the enthalpy in actual state. Thus, the mechanical power consumption can be calculated as

$$W_{\text{mch}} = \frac{\dot{m}(h_{\text{out},s} - h_{\text{in}})}{\eta_s}. \tag{26}$$

The compressed syngas flow is then mixed with compressed air in a mixer. It is assumed that there is no mass loss in the mixer. According to the energy balance, the following equation can be obtained:

$$\sum_{\text{input}} \dot{m}_{\text{in}}h_{\text{in}} = \dot{m}_{\text{out}}h_{\text{out}}.$$ \tag{27}

The mixed syngas and air will then be ignited in the combustion chamber, where the fuel gas combustion will take place, and the chemical reactions considered include

$$2H_2 + O_2 \rightleftharpoons 2H_2O, \tag{28}$$

$$2CO + O_2 \rightleftharpoons 2CO_2. \tag{29}$$

The dominant reaction in the chamber is hydrogen combustion. The remaining carbon monoxide combustion is also considered. After passing the WGS, the CO mole content in shifted syngas will drop to less than 2.47% (Karmarkar, 2005); thus, the influence of CO combustion is tenuous.

The heat generation of the combustion will be calculated by hydrogen and carbon monoxide lower heating value (LHV) as 120 and 10.112 MJ/kg. In this model, a reactor block like WGS reactor is adopted to simulate the combustion, and the reaction rate is defined as 1, which means complete combustion happens inside the chamber.

The high-temperature and high-pressure flue gas is then injected into the turbine block. The turbine can decrease the pressure of the incoming flow to a given outlet pressure. It determines the thermodynamic state of the outgoing flow along with the produced mechanical power at a given isentropic efficiency, which is similar to that of the isentropic compressor. The mechanical power generated by the turbine can be calculated by the following equations:

$$\eta_s = \frac{h_{\text{in}} - h_{\text{out}}}{h_{\text{in}} - h_{\text{out},s}}, \tag{30}$$

$$W_{\text{mch}} = \dot{m}(h_{\text{in}} - h_{\text{out},s})\eta_s. \tag{31}$$

The parameters with subscript $s$ are isentropic state change. This turbine block is defined as passive, which means the mass flow rate remains unchanged during the calculation. The isentropic efficiency used in this block is retrieved from a lookup table as a function of the mass flow. It is defined as the ratio of actual enthalpy difference to enthalpy difference for isentropic change of state with the same pressure drop. In this study, the value of isentropic efficiency is set as 0.8.

The thermodynamic characteristics of the syngas flow and flue gas flow and the mechanical power-generation
results are obtained. The thermal efficiency is calculated based on the fuel heat value and gas turbine net power generation.

6. The HRSG description

The HRSG unit is based on the Rankine cycle (Wong, 2012). It has a heat exchanger to pick up the waste heat of the flue gas to heat the feed water and generate steam. Then, the vapour will drive the turbine and then the generator to produce electricity. Using the HRSG, the thermal efficiency of the power cycle can be improved.

A pump module is adopted to provide feed water to the heat exchanger. The pump increases the pressure of the incoming water flow to target pressure. It determines the thermodynamic state of the outgoing flow along with the required mechanical power consumption. The energy balance of the compression process in the pump is calculated using the following equation (32):

\[ \dot{m} (h_{in} + \frac{1}{2}v_{in}^2) = \dot{m} (h_{out} + \frac{1}{2}v_{out}^2) + W_{mch}, \] (32)

while

\[ \dot{m} (h_{out} - h_{in}) = \frac{P_{out} - P_{in}}{\rho}, \] (33)

where \( P_{out} \) and \( P_{in} \) are the pressure of the pump outlet and inlet. \( \rho \) is density of the working flow. The power consumption is calculated by

\[ W_{mch} = \dot{m} \Delta P \eta_{pump}, \] (34)

where \( \eta_{pump} \) is the pump efficiency and is set as 0.8. The power consumption of the pump is considered in the total HRSG output calculation. With the mechanical power, the enthalpy of the water outlet is equal to the sum of input enthalpy and electric power:

\[ H_{out} = H_{in} + W_{mch}. \] (35)

The pumped feed water is then transported to the heat exchanger, where its temperature will rise to the target by adsorbing heat from the flue gas generated by the gas turbine. A heat exchanger module based on Thermolib is used for calculating the heat transfer between the flue gas and the water stream. It is important to notice that the heat transfer between these two streams is indirect and they are treated as counter flow. The two media state dynamic change will be simulated by using the number of transfer units method (Incropera & DeWitt, 1985). The actual heat transfer rate can be determined by calculating the effectiveness \( \varepsilon \), which is the actual heat transfer divided by the maximum possible heat transfer.

\[ \varepsilon = \left( \frac{Q}{Q_{max}} \right). \] (36)

For counter flow:

\[ \varepsilon = \left( \frac{1 - \exp(-M(1 - C))}{1 - C \times \exp(-M(1 - C))} \right), \] (37)

where

\[ M = \frac{UA}{\dot{C}_{min}}, \] (38)

\[ C = \frac{\dot{C}_{min}}{\dot{C}_{max}}, \] (39)

\[ \dot{C}_{min} = \min(\dot{m}_{1}c_{p1}, \dot{m}_{2}c_{p2}), \] (40)

\[ \dot{C}_{max} = \max(\dot{m}_{1}c_{p1}, \dot{m}_{2}c_{p2}), \] (41)

Figure 3. Schematic diagram of process simulation.
where $U$ is the overall heat transfer coefficient, $A$ is the surface area available for the heat transfer and thus $UA$ is the overall heat transfer rate. It represents the heat transfer between the flow and wall as well as the heat conduction in the wall. This is the product of heat transfer coefficient and effective heat exchange area between the flows.

Using the aforementioned equations (36–41), we can have

$$Q_{\text{max}} = \dot{C}_{\text{min}} (T_{hi} - T_{ci}), \quad (42)$$

where $T_{hi}$ is the temperature of the hot fluid input to the heat exchanger and $T_{ci}$ is the cold fluid input temperature. In the calculation of this heat exchanger block, the heat exchanges of both the flow streams with environment and pressure loss of the flows are considered.

The heated water steam is then injected to the steam turbine block, where the isentropic expansion process happens. The same block as described in the gas turbine system introduction is adopted for the steam turbine. The net power output of the whole HRSG system will be the difference between steam turbine power generation and pump power consumption. The dynamic change in net power of HRSG and the gas turbine system is obtained and analysed as the power output of the combined cycle.

### 7. Air separation unit

The air separation unit (ASU) is an important part in the IGCC power plants using oxygen-feed gasifiers (Wang et al., 2013). Air is liquefied and separated into oxygen and nitrogen along with some by-products such as helium. The generated oxygen is then compressed to 40 bar and injected into the gasifier for raw syngas production. Some plants integrate ASU with gas turbine, using nitrogen for combustion diluent aiming to reduce NO\textsubscript{x} emission (Karmarkar, 2005). In this paper, only hydrogen and carbon monoxide combustion are considered in the gas turbine module, the integration of ASU and gas turbine will not be included.

The working principle of ASU in this study is based on the Linde–Hampson cycle (Timmerhaus & Reed, 2007). Air is isothermally compressed first and then passes the main heat exchanger; the isobaric heat transfer between the air phase and liquid phase results in huge temperature drop. After the isenthalpic expansion process in the throttle valve, the air will be liquefied and transported to the distillation tower for further separation. In the separation process, liquid nitrogen will reach boiling point first and be separated, and pure nitrogen and oxygen will be generated for the IGCC process.

A polytropic compressor in Thermolib is adopted to simulate the isothermal process. The power consumption is calculated by using the following equation:

$$W_{\text{mch}} = n \frac{(p_{\text{out}} v_{\text{out}} - p_{\text{in}} v_{\text{in}})}{1 - n} \quad (43)$$

### Table 1. Model input.

| Input                        | Unit     | Illinois No. 6 | Australia | Fluid coke |
|------------------------------|----------|----------------|-----------|------------|
| Slurry flow rate             | kg/s     | 1              | 1         | 1          |
| Slurry concentration         | kg coal/kg slurry | 0.665    | 0.621     | 0.606      |
| O\textsubscript{2} purity   | Vol%     | 98             | 99.6      | 100        |
| O\textsubscript{2}/coal      | kg O\textsubscript{2}/kg dry coal (no ash) | 0.86   | 0.87      | 1.03       |
| Ar/O\textsubscript{2}        | kg Ar/kg O\textsubscript{2} | 0        | 0         | 0          |
| Gasifier pressure            | MPa      | 4.083          | 4.083     | 4.083      |
| Temp.                        | °C       | 1141           | 1044      | 1060       |
| Heat loss                    | H.H.V.%  | 2              | 2         | 2          |
| Ultimate analysis (dry)      | %        | 69.6           | 66.8      | 86         |

### Table 2. Comparison of the simulation results and reference data.

| Fluid | R (%) | S (%) | R (%) | S (%) | R (%) | S (%) |
|-------|-------|-------|-------|-------|-------|-------|
| CO    | 41.0  | 41.0  | 35.2  | 35.4  | 47.1  | 47.2  |
| H\textsubscript{2} | 29.80 | 30.1  | 29.9  | 29.6  | 24.3  | 23.7  |
| CO\textsubscript{2} | 10.2  | 10.0  | 12.8  | 12.8  | 13.2  | 13.3  |
| H\textsubscript{2}O | 17.1  | 16.8  | 20.3  | 20.0  | 12.7  | 13.0  |
| CH\textsubscript{4} | 0.3   | 0.15  | 0.02  | 0.22  | 0.09  | 0.33  |
| N\textsubscript{2} | 0.80  | 0.9   | 0.63  | 0.63  | 0.4   | 0.3   |
| H\textsubscript{2}S | 1.1   | 1.01  | 1.14  | 1.10  | 2.2   | 2.07  |
| COS   | 0.04  | 0.25  | 0.10  | 0.10  |       |       |
| Error | 0.26  | 0.14  | 0.21  |       |       |       |

### Table 3. Model input.

| Input                        | Unit     | Data |
|------------------------------|----------|------|
| Slurry rate                  | t/d      | 650  |
| Slurry concentration         | kg coal/kg slurry | 0.66  |
| Oxygen purity                | Vol%     | 98   |
| Oxygen/coal                  | kg O\textsubscript{2}/kg dry coal (no ash) | 0.96  |
| Pressure                     | MPa      | 4.0  |
| Temperature                  | °C       | 1350 |
| Heat loss                    | H.H.V.%  | 2    |
| Ultimate analysis            | %        | 71.5 |
| C                            | %        | 4.97 |
| H                            | %        | 11.15|
| O                            | %        | 1.07 |
| N                            | %        | 2.16 |
| S                            | %        | 9.15 |

The working principle of ASU in this study is based on the Linde–Hampson cycle (Timmerhaus & Reed, 2007). Air is isothermally compressed first and then passes the main heat exchanger; the isobaric heat transfer between the air phase and liquid phase results in huge temperature drop. After the isenthalpic expansion process in the throttle valve, the air will be liquefied and transported to the distillation tower for further separation. In the separation process, liquid nitrogen will reach boiling point first and be separated, and pure nitrogen and oxygen will be generated for the IGCC process.

A polytropic compressor in Thermolib is adopted to simulate the isothermal process. The power consumption is calculated by using the following equation:
Table 4. Comparison of dry syngas output content and industry data.

|       | CO   | H₂   | CO₂  | CH₄ + Sulphide + N₂ + Ar |
|-------|------|------|------|--------------------------|
| Industry | 48.82| 36.58| 14.41| 0.19                     |
| Simulation | 49.54| 35.69| 12.79| 1.98                     |

Figure 4. Syngas content change with coal slurry concentration unit (kg/kg).

where \( p, v \) are the pressure and volume value of different states, and \( n \) is the coefficient in the polytrophic process. The value of \( n \) in this study is set as 0.997 to stabilize the air temperature, which is required for isothermal condition.

In the isobaric heat exchanger, the gas phase air temperature is reduced to the target, and the difference in enthalpy between the input and output states is the transferred heat.

The throttle valve module is based on the Joule–Thompson effect (Perry & Green, 1984), and liquefaction of the air which has been cooled enough consists of an isenthalpic expansion. The pressure loss over the valve is calculated by the Thermolib valve block. This isenthalpic process will cause full liquefaction of the air. The valve block is based on the following equations:

\[
H_{\text{out}} = H_{\text{in}}, \tag{44}
\]

\[
\dot{m}_{\text{out}} = \dot{m}_{\text{in}}, \tag{45}
\]

\[
p_{\text{out}} = p_{\text{in}} - k(\text{pos})\dot{m}, \tag{46}
\]

where \( k(\text{pos}) \) is the function of valve position. The value is calculated based on a well-validated lookup table in the Thermolib toolbox.

In this study, the liquefied air temperature is 70 K (Kar-markar, 2005). The liquid phase air is than fractionally distilled to generate pure nitrogen and oxygen. The media flow in the model is set as a vector carrying the state parameters, which include flow rate, temperature, pressure, enthalpy, entropy, contents concentration and gas phase fraction.

8. Results and discussion

The whole process model implemented in Simulink and Thermolib is shown in Figure 3. Three types of coal are applied to test the working process of the model. The model input variables and model parameters are listed in Table 1. The simulation results of the final steady state and their associated reference data (Watkinson et al., 1991) are given in Table 2. For error analysis, the mean absolute error between the simulation results and reference data is given in Table 2.

Figure 5. Syngas content change with coal slurry concentration unit (kg/kg).
Column R denotes the reference data of syngas contents concentration in mole percentage, the column S presents the simulation results of three coal types. The comparison in Table 2 shows that the simulation results match well with the reference data (Watkinson et al., 1991).

The gasifier simulation results are then compared with the reference data from the Lu-nan fertilizer factory. The model input data are given in Table 3. Comparison of the predicted output dry syngas content results and industry data is given in Table 4.

Table 4 shows that the simulation results can match well with the industry data. This means that the assumptions and the mathematic model used in the modelling work are reasonable.
To further test the model, the change in oxygen/coal ratio and slurry concentration’s effects on the syngas content are studied. Figures 4 and 5 show the slurry concentration’s effect on syngas contents. When the slurry concentration increases from 60% to 66%, the CO content increases; while H2 remains stable, CO2 and CH4 decrease. When slurry concentration increases, more coal feed enters the gasifier; but when the oxygen/coal ratio remains stable, it means the oxygen input will rise as well, thus enhancing the gasification process and inducing content change. The results well match with Azuhata’s experiment (Azuhata, Hedman, & Smoot, 1986).

Figures 6 and 7 show the syngas content change with oxygen/coal ratio. The rise in this ratio means increase in the oxygen supply, which will enhance the combustion and raise the gasifier temperature, thus enhancing the gasification process. But it will also consume more CO and H2 released from the volatile, resulting in the decrease in CO and H2 content and the increase in CO2 content. The results match with Azuhata’s experiment (Azuhata et al., 1986) and Vamvuka’s simulation results (Vamvuka, Woodburn, & Senior, 1995a, 1995b).

Three different types of coal are applied to the simulation to test the process dynamic response. The coal feeding...
is the input of the whole system. In this test, the coal flow rate will be inputted to the gasifier model and simulated to generate syngas output. The syngas flow rises from 0.1 to 100 mol/s within 100 s and it will first enter the WGS module for shift reaction.

The concentration of CO\(_2\) and H\(_2\) and the temperature of the shifted syngas are shown in Figures 8–10.

For the three types of coal, a similar trend is observed for the dynamic change in CO\(_2\), H\(_2\) concentration and syngas temperature. The simulation results prove that the WGS module can enhance the H\(_2\) and CO\(_2\) extraction; the carbon sequestration and hydrogen combustion process will thus benefit from it. Meanwhile, the shift reaction is exothermic, and the temperature of the shifted syngas rises in the WGS. In a real power plant, the heat can be used to raise HP steam to HRSG, but in this study, the heat recovery process is not considered.

The dynamic behaviours of the gas turbine power output are shown in Figure 11, while the net power output of the combined cycle is shown in Figure 12. The power consumptions of the compressors coupled with turbines are considered.

The power outputs of the gas turbine and combined cycle show similar trends for the three types of coal. The thermal efficiency of the gas turbine cycle is 30–33%. Integrated with HRSG, the combined cycle thermal efficiency is 51–55%. Hence, the HRSG is important in improving the power generation of the IGCC process.

For the ASU module, the liquefied air flow rate is set as 150 mol/s, which can satisfy the demand for the Texaco
gasifier use based on the model input oxygen/dry coal ratio. The compressor consumption dynamic change is shown in Figure 13. In this paper, the power consumption of air liquefaction process is mainly caused by compressor usage.

In this model, pure oxygen and wet air are used as the oxidant in the gasifier and the gas turbine, respectively. In the real industry, the ASU will not only provide oxygen to the gasifier but also integrate with the gas turbine; but in this paper, since NOx is not considered as the combustion product, integration of the ASU and the gas turbine is not included.

9. Conclusion

In this paper, a mathematical model for an IGCC process using Taxaco gasifier is developed which can predict the syngas contents. The model is derived by applying the engineering principle, the chemical equilibrium, mass balance and energy balance. The simulation results of dry syngas match well with the industry data. The influence of coal slurry concentration and oxygen/coal ratio on the syngas contents is studied as CO, CO2 and H2 contents of coal slurry concentration and oxygen supply is shown to be one of the suitable solutions. The dynamic behaviour of WGS shows its importance in improving syngas quality potential to heat steam. To improve the syngas quality and prepare for further carbon capture, WGS plays a key role. HRSG improves the thermal efficiency of the combined cycle and the overall power-generation process. ASU can lead to efficiency loss of the whole power plant since the liquefaction and transportation processes will both consume a large amount of energy.

Disclosure statement

No potential conflict of interest was reported by the authors.

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