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Process simulation of the transport gasifier

Christopher J. Arthur, M.T. Munir, Brent R. Young, Wei Yu *

Industrial Information and Control Centre (I^2C^2), Department of Chemical and Materials Engineering, The University of Auckland, Auckland 1010, New Zealand

HIGHLIGHTS

- A KBR transport gasifier has been successfully simulated.
- Three alternate process simulation models were developed.
- Gibbs free energy based model performed the best among the three models.
- Models were validated using real data (i.e. KBR data).

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ABSTRACT

The transport gasifier manufactured by Kellogg, Brown and Root (KBR) is reportedly capable of economically converting low rank coal (e.g. lignite) to syngas for the production of synthetic chemicals, fuels and energy. However no process simulation of the KBR transport gasifier yet exists in the public domain literature. In this work three alternative process simulation models of the transport gasifier were developed using a commercial process simulator combined with Excel/VBA routines. The first model determined gasification products on the basis of minimum Gibbs energy. The second model used pseudo-equilibrium approach and the third model used kinetic expressions. The simulation models were validated with real process data. The pseudo-equilibrium model was best able to replicate the data with reasonable process assumptions.

1. Introduction

Lignite is a low rank, low value coal that is abundant in New Zealand [3,32,19]. It is unsuitable for conventional combustion as it has a low heat of combustion relative to higher ranks of coal. However Lignite is particularly suited to gasification, with the right technology, due to its high reactivity. High coal reactivity will allow a gasifier that can operate at a lower temperature to be used in a process. The reduced cost of the refractory will increase the economic case [12].

The transport gasifier manufactured by Kellogg, Brown and Root (KBR) typically operates at temperatures 520 °C cooler than the market leading Shell coal gasification process [12] and is particularly suited to lignite [16,17]. No process simulation for the KBR transport gasifier exists in the public domain literature.

The transport gasifier is a recent technology and independent sources describing the gasification reactor include Higman and Burgt [12], Rezaiyan and Cheremisinoff [21] and Bell et al. [4] where complimentary accounts are given. The gasification reactor is described as having a carbon conversion of approximately 95% making the assumption that carbon reacts to completion simplistic. It is notable that different coal ranks have a large effect on process outcome. A more detailed publically available description of the transport gasifier is given by Mann et al. [16]. The review states that the transport gasifier does not expose fresh coal to the oxidant. Re-circulated char is the source of combustion heat not volatiles. This has important implications when defining the simulation topology. However the review is qualitative and reveals few quantitative performance attributes.

The transport gasifier operates at relatively low temperatures, making kinetic considerations important. A key publication by Mann et al. [16] considered the char reaction kinetics in a transport gasifier. It was concluded that the reaction of char with steam was the dominant carbon reaction and an Eq. (1) was presented that can determine the conversion rate of carbon in the transport gasifier due to steam gasification.

$$\frac{dX}{d\tau} = 1.4 \times 10^7 \times e^{\frac{-2\times10^4}{T}} \times P_{H_2O}^{0.63} \times P_{Total}^{-0.7} \times \left(\frac{CO}{CO + CO_2}\right)^{-1.91} \quad (1)$$

where X is the carbon fraction, P the pressure (atm), T the temperature (K), τ is the residence time (min).

Eq. (1) will allow a model to determine the carbon conversion if the residence time is known. However the equation was designed

* Corresponding author. Tel.: +64 9 373 7599x85027; fax: +64 9 373 7463.
E-mail address: w.yu@auckland.ac.nz (W. Yu).

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using only three data points making the reliability difficult to assess.

The KBR transport gasifier also operates as a high velocity, circulating, fluidised bed reactor. The reactor has no internals or moving parts and is robust to various coal particle sizes. Solid char particles circulate through the reactor until converted or ejected with the ash. The high velocity circulation increases heat and mass transfer and reduces the operating temperature [12,2,20]. Operating below the agglomeration temperature of coal ash prevents refractory damage and the need for complex expansion joints, thereby reducing the capital cost [8]. A schematic of the transport gasifier can be seen in Fig. 1.

The objective of this study is to create a model using a commercial process simulator that can replicate the data provided by KBR with reasonable assumptions. A process simulation capable of predicting mass and energy flows for lignite gasification using the transport gasifier would be a useful tool to evaluate the economic case for the gasifier and to assess sensitivity to process variation.

Previous studies into the gasification of coal gave a critical insight into the capabilities and limitations of process modelling and the assumptions included in the models. No process models were found that considered the KBR transport gasifier. A selection of the other previous gasification models are presented below.

Nathen et al. [18] created a model of the Shell gasifier using the process simulator HYSYS. The coal was modelled as a ratio of carbon, water and methane and Gibbs energy minimisation formed the basis of determining the products. Nathen et al. [18] also assumed that the char reacted to completion, that the gasifier is adiabatic, that equilibrium conditions were achieved quickly and slagging of the coal ash required no energy. These assumptions will have to be addressed to differentiate between gasifiers. The model could not account for kinetic limitations. A coal analysis with greater resolution would be beneficial to a gasification model for chemical production as impurities in the syngas, particularly sulphates, affect downstream units [7].

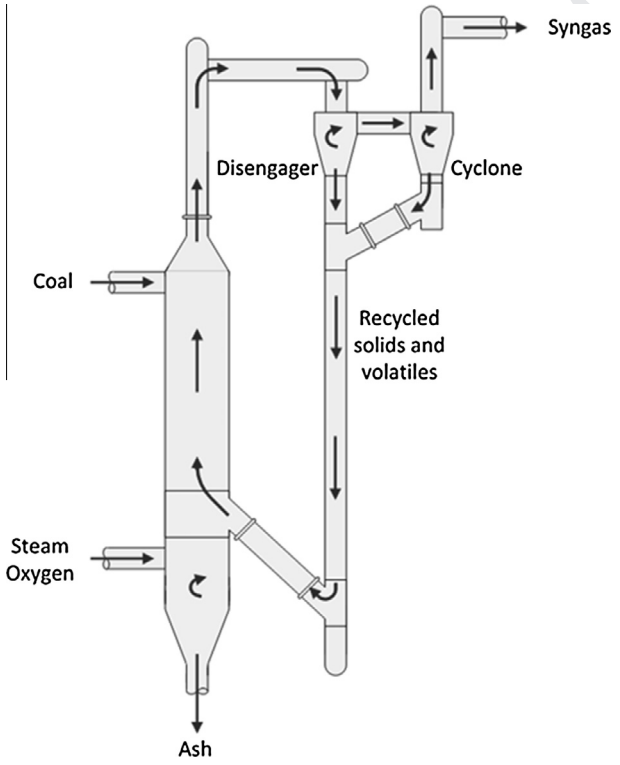

Fig. 1. Transport gasifier schematic illustrating the circulating fluidised bed.

Gnanapragasam et al. [11] also used Gibbs energy minimisation but using an ASPEN PLUS® simulation platform. Heat loss was evaluated in the model and species stable above 873 K were included. Gnanapragasam et al. [11] also assumed all char was reacted and that there was no kinetic limitation. In the model nitrates formed molecular nitrogen whereas ammonia and hydrogen cyanide are coal gasification products and generally of higher concentrations [12].

Ardila et al. [1] used a Gibbs energy minimisation simulator nested within a recycle loop in ASPEN PLUS® to simulate a circulating fluidised bed gasifier. The simulation demonstrated that using a yield reactor to convert solid components to specified products based on an ultimate analysis is a legitimate way of simulating pyrolysis. The simulation assumed that there was no kinetic limitation to gasification.

Kunze and Spliethoff [15] considered kinetic limitation in an ASPEN PLUS® gasification model by defining gasification as a series of linearly-independent reactions and specifying a temperature approach to equilibrium for each reaction. The model was able to closely replicate empirical results. Departure from equilibrium was specified to fit a known output. The approach temperatures were not published.

A report by Kramer [14] for the United States Department of Energy published an ASPEN PLUS® simulation with specified approach temperatures. The results showed significant departures from thermodynamic equilibrium for the reaction of char with hydrogen and the water gas shift reaction. The model could simulate gasification with a high level of accuracy but the approach temperatures did not have a theoretical basis.

An introduction to "net flow" concept and how it can affect the hydrodynamics in a gasifier has also been analysed [33,34]. From these reported studies, it was concluded that the simulation results without the net flow concept can deviate significantly from the practical results.

This manuscript is organised as follows. After this general introduction, the materials and methods used in this work are explained and discussed in Section 2. In Section 3 simulation methodology is explained. In Section 4 results are discussed. Finally in Section 5 results are summarized, limitations are discussed, and conclusions are made.

2. Materials and methods

2.1. Coal classification

The transport gasifier is suited to young coals particularly lignite. Coal rank with increasing geochemical maturity is shown in Fig. 2 [5]. Lignite is the lowest rank of coal and the boundary between lignite and peat is unclear. Lignite resembles its original plant matter to a greater extent than mature coals. Lignite is porous and contains high fractions of oxygen and therefore functional groups that affect reactivity. Relative to higher ranks, lignite has a smaller proportion of aromatic carbon atoms, approximately half of the total carbon, and a greater hydrogen content, approximately 1:1 (mole:mole) hydrogen to carbon [13,26].

2.2. Coal gasification

Generally, gasification is the conversion of a carbonaceous feedstock to a gas with a thermal heating value [12,17]. Gasification differs from combustion as combustion products have no thermal value. The gasification process can include: (i) pyrolysis; (ii) partial oxidation; (iii) char reactions; and (iv) gas phase reactions.