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Process behavior of extra-heavy oil gasification under different fuel water contents

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HIGHLIGHTS

- A kinetic model for extra-heavy oil is developed.
- The effect of some critical parameters on system performance is studied.
- Model predictions are compared against available data from the literature.

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ABSTRACT

In this study, a kinetic model for extra-heavy oil gasification has been developed. It is a zero dimensional, steady state model based on global reaction kinetics and is capable of predicting performance parameters of the process. Effects of parameters, including fuel water content and equivalence ratio on tar yield, gasification temperature and performance parameters such as syngas higher heating value (HHV), carbon conversion efficiency (CCE), cold gas efficiency (CGE) have been discussed. The results indicate that the higher equivalence ratio is more favorable for carbon conversion and tar cracking; however, it lowered gas caloric value and cold gas efficiency. It is also found that the higher carbon conversion and lower tar yield are possible at higher fuel water content. The model is validated by experimental and thermodynamic data and found relatively to be in good agreement.

1. Introduction

Oil is the major energy resource and it will held this role in near future. Quality of crude oil decreases and its sulfur content increases gradually and it becomes heavier [1]. Therefore, increasing heavy and extra heavy oil and subsequently increasing heavy refinery residue in one hand, and increase in demand for middle distillate products and environmental issues on the other hand, make the development of efficient and environmentally friendly upgrading technologies necessary. Gasification, as a thermochemical process to convert carbonaceous materials to syngas, is an interesting alternative technology for energy recovery from various feedstocks [2]. Also, combination of gasification with other heavy oil upgrading technologies can be interesting [3]. Several systems using heavy oil gasification for different purposes are studied and seemed to be attractive from environmental and/or economical viewpoints [4–7]. Because of these advantageous, several petroleum refinery worldwide use gasification process [1].

Gasifier is the most important part of gasification systems and its performance affects the efficiency of gasification system. Performance of a gasifier is influenced by several parameters such as feedstock property, gasifier geometry, temperature, pressure and so on. Although gasifier geometry and property of input feedstock are relatively important, the performance of a gasifier is directly influenced by the choice of operating conditions such as equivalence ratio, pressure, and gasifying agent. Many researchers are studied the effects of these parameters on gasification performance for different feedstocks, either experimentally [8–10] or by modeling [11–13]. However, studies on gasification of heavy and extra heavy oil and petroleum residue are not abundant. Ashizawa et al. investigated Orimulsion gasification experimentally in a 2.4 t/d entrained flow gasifier [14]. Gasification of vacuum residue in an entrained flow gasifier carried on by Choi et al. [15]. Experimental studies are important and insightful to understand the process. However due to their difficulties and cost, modeling of gasification is used extensively to investigate different aspects of this process.

Two approaches are used to model gasification process; equilibrium and kinetic. These two approaches have some advantages and drawbacks. The equilibrium model loses some details of process

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while kinetic model needs more inputs and are more complicated. Vaezi et al. employed thermodynamic equilibrium model to study the effects of equivalence ratio, oxygen enrichment and pressure on syngas composition, carbon conversion, and gasifier efficiency in Orimulsion gasification [16]. The assumption of chemical equilibrium is not valid for most of the processes and equilibrium model predictions are not always accurate enough. Therefore, some researchers used more detailed kinetic and CFD models to study gasification of heavy oils. A CFD simulation of heavy oil gasification in an entrained flow gasifier is developed to illustrate syngas composition and temperature along reactor axis [17]. Watanabe et al. elucidated the effects of oxygen ratio on syngas composition and temperature by a detailed kinetic and 3D model [18]. Gasification of asphalt, as a petroleum residue, in water slurry in a entrained flow gasifier is investigated by Xingying et al. [19]. A three-dimensional CFD simulation is developed to investigate pitch-water slurry gasification in two types of gasifiers [20]. These CFD analyses of gasification are more complicated to achieve a general perspective of the gasification process. Therefore, a need for a kinetically detailed but simple model which describe the gasification process of petroleum hydrocarbons is felt.

In this paper, a zero-dimensional kinetic model for heavy oil gasification is developed. It also addresses the complex phenomena that occur during the gasification process such as tar formation, which most research papers fail to cover; in lieu of what is discussed. After comparing the model predictions with available experimental data, results are discussed.

2. Modeling approach

2.1. Fuel properties

Orimulsion is used in this study as a heavy oil. Orimulsion is a bitumen-in-water emulsified fuel extracted from a large oil field located in Eastern Venezuela, which is recently well recognized as an energy source for power generation in Italy, Canada, Japan, Lithuania, Denmark, and UK [21]. In recent years, Orimulsion has also been proposed as a fuel for utility and industrial boilers, diesel engines, and cement kilns, due to a rather low price in comparison to other fuels [22]. The molecular formula of dry ash-free Orimulsion ($CH_{1.4651}O_{0.6782}N_{0.0007}$) is calculated based on the average ultimate analysis of fuel which investigated by Ashizawa et al. [14] as presented in Table 1.

2.2. Process assumptions

A simplified process is considered to predict the performance characteristics of heavy oil gasification, using air as gasification agent. The main assumptions regarding gasification process in present model are listed as follows: (i) the syngas is comprised of H_2, CO, CO_2, H_2O, CH_4, and C_2H_4 (ii) to solve mass balance equation, the product yields calculated in the pyrolysis step is used as initial conditions in the gasification step; (iii) char is modeled with the only component of carbon black; (iv) it is assumed that the gasifier operates under steady state conditions and atmospheric pressure; (v) the thermal conductivity of gas mixture is calculated using the Wilke–Eucken equation [23]; (vi) ash is assumed to be chemically inert under the studied conditions because the kinetic data about chemical properties of ash were not found in the literature; (vii) it is assumed that the reactor performance is insensitive to the hydrodynamic properties; (vii) the heat loss has also been assumed as 1% of the overall heat released.

Table 1
Properties of Orimulsion [3].

Proximate analysis		Ultimate analysis (dry)	
Water	28.80%	C	84.28%
Ash	0.18%	H	10.33%
Residual carbon	12.84%	O	0.55%
Total sulfur	2.81%	N	0.64%
HHV (MJ/kg)	29.76	S	3.95%
		Ash	0.25%

2.3. Devolatilization

Devolatilization is an extremely complex reaction that can ideally be defined as thermal decomposition of the fuel in the absence of an oxidizing agent. Although the devolatilization usually takes place instantaneously (due to high temperature), a lot of effort has been made to model gasification step with respect to the concentration of the products in the pyrolysis step. Maki and Miura [24] measured the devolatilization yields using the same fuel in this study in an entrained bed reactor within the temperature range of 500–1200 °C. They used special tar and syngas sampling device to measure tar and gas amount and composition. The details of the experimental setup can be found elsewhere [24].

2.4. Model formulation

A steady state, zero-dimensional model is developed to simulate air-gasification of heavy oil. Similar approach has been used by Inayat et al. [25] for a process modeling work on biomass steam-gasification with in-situ CO_2 capture. The mass and energy balance between the reactants and products can be calculated based on the following equations

$$\sum_{i=react} m_i = \sum_{j=prod} m_j \tag{2.1}$$

$$\sum_{i=react} n_i(H^\circ_{f,i} + \Delta H^\circ_{T,i}) - \sum_{j=prod} n_j(H^\circ_{f,j} + \Delta H^\circ_{T,j}) + Q_{loss} = Q_r \tag{2.2}$$

$$\Delta H^\circ_T = H^\circ(T) - H^\circ(298) = \int_{298}^{T} C_P(T)dT \tag{2.3}$$

where $\sum_{i=react} m_i$ and $\sum_{j=prod} m_j$ are the mass flow rates of input and output material stream respectively, ΔH°_T is the enthalpy change in J/h which is calculated based on the heat capacities, C_P is the specific heat at the constant pressure in J/mol K, Q_{loss} is the heat loss in J/h, and Q_r is the heat of reaction in J/h. The material mass balances inside the control volume are checked by the stoichiometry of the reactions involved. Enthalpy change is calculated using heat capacities. The heat capacity of each species at a specific temperature is calculated based on the following formula [26]:

$$\frac{\overline{C}_p(T)}{R} = n_1 + n_2T + n_3T^2 + n_4T^3 + n_5T^4 \tag{2.4}$$

where coefficients of this equation are available for several species [26]. The enthalpy of formation of fuel is expressed as a function of the number of complete combustion species based on De Souza-Santos relation, which given as [27]

$$H^\circ_{f,\text{fuel}} = \text{LHV}_{fuel} + \frac{1}{M_{fuel}} \sum_{k=prod} n_k (H^\circ_f)_k \tag{2.5}$$

Here LHV is the lower heating value of the feedstock in kJ/kmol, M_{fuel} is the molecular mass of the feedstock in gram. For calculating the HHV of the fuel, which is the basis for obtaining the LHV, empirical correlation of Channiwala–Parikh [28] is used, as follows:

$$\text{HHV} = 0.3491\text{C} + 1.1783\text{H} + 0.1005\text{S} - 0.1034\text{O} - 0.0151\text{N} - 0.0211\text{A} \tag{2.6}$$

Here C, H, S, O, N, and A are mass fraction of carbon, hydrogen, sulfur, oxygen, nitrogen, and ash in dry feedstock, respectively. The

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