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Modeling of the entrained flow gasification: Kinetics-based ASPEN Plus model

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In this study, the entrained flow gasification (EFG) of Kentucky coal and wood waste had been investigated using detailed kinetics-based ASPEN Plus model and experimental diagnostics. The experimental investigation was conducted in the air-blown atmospheric drop tube experimental facility furnace. The exit gas composition at different equivalence ratios was obtained to validate the developed ASPEN Plus model. In addition, the scanning electron microscopy (SEM) images of the char were observed along the gasifier to determine the behavior of the feedstock subjected to gasification and to select proper char gasification models. The model takes into account the passive heating through moisture release, devolatilization, volatile combustion and char gasification. It made the investigation of the gasification process and running sensitivity studies practically feasible as current equilibrium and high fidelity coupled thermo-chemical-flow models are insufficient or pertaining much complexity to use. The model compares reasonably well with the experimental data obtained in this work and is been used to carry out sensitivity study. A rise in the diameter and height sizes lead to an increase in the mole fraction of CO and H_2 throughout the length of the gasifier, an opposite trend was observed for the CO_2 and H_2O composition. It was also observed that the mole fraction of the syngas was lower for the biomass waste compared to the baseline coal as this is attributed to the higher oxygen content (43.62%) and lower carbon content (49.41%) of the waste biomass compared to coal.

1. Introduction

Millions of tons of solid and biomass wastes are generated annually that continue to pose serious environmental and ecological threats to our planet. In 2009, the total amount of solid waste in the Emirate of Abu Dhabi, United Arab Emirates, was 5756 thousand tons according to the estimates of the Center of Waste Management-Abu Dhabi, with the construction sector contributing 61% of the total waste due to the construction boom taking place in the Emirate [1]. At the current population growth, development and industrialization, this trend would tend to intensify. However, majority of these construction wastes are wood which end up in landfills and causes havoc to the environment. This waste stream along with other MSW, if segregated and properly treated can be gasified instead, to generate syngas of high economic value, thereby solving the problems of waste management, carbon emission, and contributing to the renewable energy emirate mandate (7% by 2020).

Although there are some equilibrium-based ASPEN Plus models for EFGs [2–10], there are very few studies on the detailed kinetics-based ASPEN Plus model development [11–13,16,17] in the literature. Some of the very few kinetics-based ASPEN Plus model for gasification includes the work of Wen and Chaung [11] who developed a single-step pyrolysis model with rate expressions for the reaction of char with CO_2, O_2 and H_2 and a global rate for gaseous equilibrium. In addition, a similar model was used by Govind and Shah [12] who compared their results with experimental data from Texaco entrained-bed pilot plant gasifier for different feeds (coal liquefaction residue and coal water slurry). In another study at CSIRO, Gartner et al. [13] developed a semi-empirical kinetics-based entrained flow gasifier model in ASPEN Plus for the simulation of the gasification of ternary fuel blends (dried lignite, extraction residue and char) in air-blown pressurized entrained flow reactor (PEFR) using the pyrolysis product distribution data of Mill [14]. Their study was validated with the gasification studies for the three Australian coals, CRC252, CRC274, and

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Nomenclature

Aspen Plus operational block descriptions

RGIBB	A reactor model that uses Gibbs free energy minimization to solve multiphase chemical equilibrium
RSTOIC	A stoichiometric reactor model with a specified reaction extent of conversion
RYIELD	A non-stoichiometric reactor model with a specified yield distribution
SEP	A separator using known outlet fractions for multiple streams
MIX	A stream mixture
FSPLIT	A stream splitter
FLASH	A separator splitting the feed into two outlet streams using vapor–liquid phase equilibrium

Special character

P_i	partial pressure of the ith specie, [Pa]
P_i^*	reference pressure of the ith specie, [Pa]
R	reaction rate, [kg/m^{2}Pa.s]
r_c	radius of an unreacted-core shrinking particle, [m]
R_d	outside radius of an unreacted-core-shrinking particle, [m]
K_{dif}	gas film diffusion, [g/cm^2/Pa]
k_{ash}	ash fil diffusion coefficient, [g/cm^2/Pa]
f, x	initial and instantaneous particle conversion
$v_{i,n}$	the stoichiometric factor for the ith specie in the nth reaction

CRC299 [15]. Lee et al [16] also investigated the effects of different burner types and oxygen gas supply angle of the burner on the gas composition, carbon conversion and gasifier temperature of a bench-scale entrained flow gasifier in ASPEN Plus. They validated their model with the experimental data from the 1-ton-per-day oxygen-blown Korea Electronic Power Corporation (KEPCO) research institute gasifier. Besides these few studies, there had been no other works on the kinetic modeling of an EFG using ASPEN Plus.

This study seeks to investigate the entrained flow gasification of wood waste with ASPEN Plus model and experimental diagnostics while using Kentucky coal as a baseline. The experiment is based on the drop tube experimental facility developed at the Waste-2-Energy Laboratory at Masdar Institute [17]. The developed ASPEN Plus model utilizes the unreacted shrinking core model for the char gasification. Moreover, the model includes the moisture release, devolatilization and volatile combustion. The effect of parameters such as gasifier diameter, height and fuel type on the gas composition and gasification metrics (efficiency and conversion) was also studied.

2. Material characterization

The Kentucky coal and the wood waste collected from the MSW facilities in Abu Dhabi have been characterized using the three conventional analytical methods: Proximate, Elemental, and Bomb calorimetry. The proximate analysis is carried out using the DSC/TGA Q600 thermal analyzer; the ultimate analysis is carried out using the FLASH 2000 CHNOS analyzer; and the heating value determination is conducted using the Parr 6100 bomb calorimeter. Several collected samples are obtained and milled to 0.1 mm mesh size to ensure homogeneity and then palletized according to the need of each test. Each test is repeated five times to statistically form acceptable data measurements (see Table 1). The Kentucky coal is a bituminous coal type obtained from the River Trading Company (RTC) and the wood waste is the common phenolic film construction plywood collected from the Al Dhafra landfill in Abu Dhabi. Both feedstocks can be considered as good candidates for gasification as the fractions of the moisture and ash content are less than 10% altogether as shown in Table 1.

3. Experimental study

The atmospheric drop tube reactor (DTR) - designed at the Waste-2-Energy Laboratory at Masdar Institute- is composed basically of a stainless steel rectangular shaped furnace fitted with insulation and heating modules within the refractory wall that encapsulate the nick alloy tube. It can attain up to 1,400 K wall temperature, under regulated and controlled nitrogen and oxygen flow rate. The gasification process actually occurs when the oxidant and nitrogen gas supply system is injected into the entrained/dossed feedstock via the particle injection system. It is equipped with diagnostics tools for gas analysis and both centerline and wall temperatures. The experimental set-up and its schematic representation are depicted in Fig. 1. The furnace and tube specifications of the drop tube reactor are as depicted in Table 2.

3.1. Sample preparation

Because entrained flow gasification requires very fine particles (usually lower than 100 microns), the Kentucky coal and wood waste were grinded and sieved using Retch Zm 200 centrifugal mill into the required size. Aggregates of coal and wood as large as 100 g were crushed and sieved with the 0.4 mm ring mesh for five different batches for each of the Kentucky coal and wood waste. Thereafter, the finely crushed particles were fed into the 2nd vibratory impact laboratory test sieve in order to classify them based on the cumulative weight distribution of the particles as depicted in Fig. 2. Five sieves of mesh sizes 25, 40, 100, 250 and 400 microns were used for the classification process. Accordingly, almost 90% of the total weight was below 100 microns for both feedstocks. Hence, the entrained flow gasification experimental study can be conducted.

3.2. Experimental method

After admissible particles size had been prepared for entrained flow gasification the drop tube reactor (DTR) experiments were initiated. Firstly, the drop tube was heated under non-reactive conditions to a temperature of 1,373 K using a PID temperature controller. The PID heating program is composed of two ramps (one between 300 and 923 K for 80 min and the other between 923 and 1373 K for 80 min) and with two isothermal heating of 20 min and

Table 1
Material characterization of Kentucky coal and Waste wood.

Proximate analysis (wt. %)	Kentucky coal	Waste wood	Ultimate analysis (wt. %)	Kentucky coal	Waste wood
Moisture	2.67 ± 0.05	8.95 ± 0.05	Carbon	76.48 ± 0.07	49.41 ± 0.07
Volatile	39.58 ± 0.05	68.89 ± 0.05	Hydrogen	5.24 ± 0.07	6.26 ± 0.07
Fixed Carbon	51.12 ± 0.05	21.88 ± 0.05	Nitrogen	2.32 ± 0.07	0.39 ± 0.07
Ash	6.63 ± 0.05	0.28 ± 0.05	Oxygen	8.27 ± 0.08	43.62 ± 0.07
HHV (MJ/kg)	Kentucky Coal	Waste Wood	Sulfur	1.06 ± 0.02	0.04 ± 0.02
Value	30.42 ± 0.50	18.70 ± 0.40	Ash	6.63 ± 0.05	0.28 ± 0.05