

Co-Firing of Refinery and Wood Waste Streams in an Entrained Flow Gasifier: The Case of Petroleum Coke and Construction/Demolition Wood

Isam Janajreh ^{a*}, Idowu Adeyemi ^a

^a *Masdar Institute of Science and Technology, P. O. Box 54224, Abu Dhabi, UAE*

Abstract

In this study, a numerical model for the gasification of a mixture of Petroleum Coke as the residual of the refinery waste stream and the construction and demolition waste inside an oxygen-fed atmospheric entrained flow gasifier (EFG) was developed. Thermogravimetric analysis is carried out first to reveal their proximate compositions and thereby appropriate co-firing proportions. Three mixing percentage of petroleum coke (10%, 25% and 50%) has been considered. The two feedstock was characterized with thermo-gravimetric analyzer (TGA) for the proximate analysis, and with Flash 2000 for their elemental analysis and bomb calorimeter (Parr 6100) for the heating value determination. The high fidelity gasification model is based on the Lagrangian-Eulerian approach whereby the solid phase particles are tracked with the Lagrangian approach and the surrounding gas phase is tracked by the Eulerian phase. The model takes into account the turbulent flow for the continuous phase (Realizable k- ϵ model), gas phase gasification (Species transport model), devolatilization (Kobayashi two competing rate model), heterogeneous char reaction (Multiple surface reaction model), particle dispersion by turbulent flow (Stochastic discrete random walk model), radiation (P1) and particle distribution (Rosin rammler model). The effect of petcoke percentage, wall temperature and the particle size on gas composition and gasification metric has been studied and reported.

Keywords: EFG, Lagrangian-Eulerian, Kobayashi model, Gasification, Construction wood, Petroleum *Coke*

INTRODUCTION

1. Introduction

Petroleum coke is often difficult to utilize as a stand-alone feedstock because it is low in volatile compounds, which makes it challenging to ignite. It is therefore often blended with higher volatile feedstock such as coal so that enhances its burning characteristics. Moreover, petcoke pricing creates significant advantages for coal plants that are able to co-fire the fuel to supplement their coal supply because petcoke is quite cheap. Literature still lacks the consideration of mixture of pet coke and biomass despite the various 2-D and 3-D numerical models for the gasification of coal particles in the literature [1-4]. For example, Hampp [1] developed a 2D model for the gasification of Kentucky coal inside a drop tube reactor. Chen et al. [2] developed a 3-D simulation model for an air-blown 200-ton-per-day two stage entrained flow gasifier, with numerical methods and sub-models conventionally used for pulverized coal combustion. Watanabe et al. [3] performed multi-dimensional computational modeling of an entrained flow gasifier for coal gasification with the Lagrangian-Eulerian based approach. Abani and Ghoniem [4] developed a model for a 3-D multiphase reacting flow in a coal fed entrained flow gasifier using Large Eddy Simulation (LES) –with a one-equation eddy viscosity model- and Reynolds-averaged Navier Stokes (RANS) –with a k- ϵ model- for the gas phase turbulence. Ghenai and Janajreh [5] studied the effect of biomass (wheat straw) addition to bituminous coal on the centerline NO_x and CO₂ concentration. They discovered that the NO_x and CO₂ concentration decreased along the centerline with the addition of wheat straw. However, there has been no known study of the numerical modeling of the entrained flow gasification of the mixture of petroleum coke and demolition/construction waste in the literature.

Hence, the goal of this study is to develop a numerical model for the entrained flow gasification of the mixture of petroleum coke and construction waste using the Lagrangian-Eulerian approach. This work also focus on the optimization of the developed model via the parametric study of the effect of parameters such as the mixing ratio of petroleum coke to demolition waste wood, wall temperature and particle size on the co-fire gasification. Lope

2. Material Characterization

The material characterization of the pet coke and demolition wood was conducted at the Masdar Institute Waste to Energy Laboratory using the Thermo-Gravimetric Analyzer (TGA) for the proximate analysis and the Flash (CHNOS) analyzer for the ultimate analysis of the Pet Coke and wood waste to determine the characteristics of the mixture. The characterization gives an insight into the composition of feedstock before further analysis. While the elemental analysis is necessary to infer the chemical formula of the feedstock, molecular weight, to regulate the stoichiometry of the oxidizer/moderator gases and estimate enthalpy of reaction [7-9], the proximate analysis help in the proper selection of devolatilization, moisture release and char combustion models. The proximate and ultimate analysis data for the mixture at 10%, 25% and 50% of petroleum coke are determined. For the ultimate analysis, several samples of the pet coke and wood waste were prepared in tin capsules and placed into an oxidation-reduction reactor of temperature between 900 and 1000 °C. This causes the samples to completely combust and raising the heat in the reactor to around 1800 °C. At this high temperature, all organic and inorganic substances are converted into totally oxidized compounds which would be carried to the chromatography column and quantify their compositing according to their thermal conductivity detection (TCD).

Table 1: Ultimate analyses of petroleum coke and construction wood waste (to be updated)

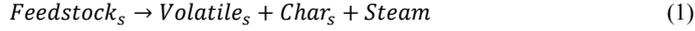
Ultimate (mass %)	Petroleum Coke (10%)	Petroleum Coke (25%)	Petroleum Coke (50%)
C	77.879	79.9775	83.475
H	5.187	5.1075	4.975
N	2.183	1.9775	1.635
O	7.573	6.5275	4.785
S	1.183	1.3675	1.675
A	5.995	5.0425	3.455
Total	100	100	100

Table 2: Proximate analyses and heating value of the petroleum coke and construction wood waste (to be updated)

Proximate (mass %)	Petroleum Coke (10%)	Petroleum Coke (25%)	Petroleum Coke (50%)
M	2.411	2.0225	1.375
V	37.106	33.395	27.21
FC	54.488	59.54	67.96
A	5.995	5.0425	3.455
Total	100	100	100
LHV (MJ/kg)	30.848	31.49	32.56

3. Model Development

The gasification of the feedstock includes moisture release, devolatilization, gas phase reactions and char combustion. These processes are expressed as .



Due to the elevated gasifier temperature, as soon as the solid feedstock/fuel is injected into a gasifier its moisture is released soon after volatiles is freed according to equation (1). The finish of the devolatilization marks the onset of char gasification reactions (equation 3-5).

a) Modeling equations

Modeling the gasification phenomenon, involves the conservation of mass, momentum, and energy as well as the participating and reacting species. These conservative laws in mathematical forms for the cylindrical with an axi-symmetrical symmetry are written as:

i) Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_x)}{\partial t} + \frac{\partial(\rho v_r)}{\partial t} + \frac{\rho v_r}{r} = S_m \quad (6)$$

Where ρ is the density and upper case S_m is the source terms due to the dispersed/discrete phase interaction.

ii) Conservation of momentum

These equations are written for the transport of the density velocity multiple vector (ρu_i) and are given axially and radially, respectively as:

$$\frac{\partial(\rho v_x)}{\partial t} + \frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x v_x) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r v_x) = -\frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(2 \frac{\partial v_x}{\partial x} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] + F_x \quad (7)$$

$$\frac{\partial(\rho v_r)}{\partial t} + \frac{1}{r} \frac{\partial}{\partial x} (r \rho v_x v_r) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r v_r) = -\frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(\frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(2 \frac{\partial v_r}{\partial r} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] - 2\mu \frac{v_r}{r^2} + \frac{2}{3} \frac{\mu}{r} (\nabla \cdot \vec{v}) + \rho \frac{v_z^2}{r} + F_r \quad (8)$$

Where p is the pressure, μ is the fluid viscosity, and F_x is the present body forces in the form of gravitational force and the divergence of the velocity is expressed as:

$$(\nabla \cdot \vec{v}) = \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} \quad (9)$$

iii) *Conservation of energy*

This equations are given for the transport of the density internal energy scalar multiple (ρE) and is written as:

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla \cdot (k_{eff} \nabla T - \sum_j h_j \vec{J}_j + (\bar{\tau}_{eff} \cdot \vec{v})) + S_h \quad (10)$$

$$E = h - \frac{p}{\rho} + \frac{v^2}{2} \quad (11)$$

$$h = \sum_j Y_j h_j \quad (12)$$

Where E is the internal energy, K_{eff} is the effective conductivity, h is the enthalpy and Y_i is the mass fraction. S_h is any external energy source that is unaccounted for.

iv) *Conservation of species:*

These are the transportation of each participating species from the reactant and product of each reactions and are given in their generic form as:

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (13)$$

Where R_i is the addition or the destruction of the species due to the reaction as is expressed as:

$$R_{j,r} = R_{kin,r} (p_n - \frac{R_{j,r}}{D_{0,r}})^N \quad (14)$$

Where $R_{kin,r}$ is the Arrhenius reaction rate written as:

$$R_{kin,r} = A_r T_p^{\beta r} e^{-(E_r/RT_p)} \quad (15)$$

And D_o is the effective surface area which is function of the localized temperature and particle diameter and is written as:

$$D_{0,r} = C_{1,r} \frac{[(T_p + T_\infty)/2]^{0.75}}{d_p} \quad (16)$$

The discrete Phase Model Equations are expressed as:

$$\frac{du_p}{dt} = F_D (u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad (17)$$

With F_D the drag force and Re particle Reynolds number and are expressed as:

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re}{24} \quad (18)$$

$$Re = \frac{\rho d_p |u_p - u|}{\mu} \quad (19)$$

Where $F_D (u - u_p)$ is the drag force per unit particle mass, u is the fluid phase velocity and u_p is the particle velocity; ρ is the fluid density, and ρ_p is the density of the particle. Equation (17) incorporates additional forces (F) in the particle force balance that can be important (thermophoretic and Brownian forces).

b) Model setup and boundary conditions

The geometry and baseline mesh of the laboratory scale gasifier is depicted in Fig. 1 with detailed dimension as well as the boundary conditions.

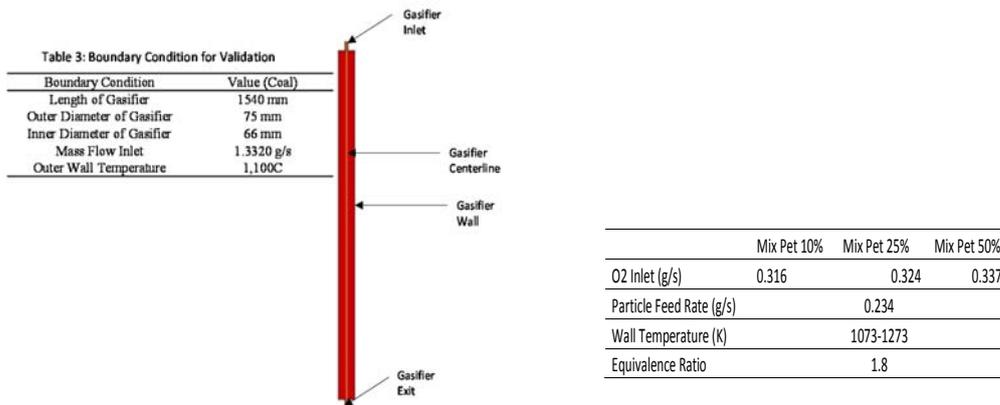


Fig. 1: Geometry and baseline mesh setup and boundary conditions

c) Solution Approach and Model Validation

The numerical model of the gasification processes in the entrained flow gasifier was conducted within the Ansys Fluent platform. Fig. 4 depicts the different implemented models. It is a combination of the Eulerian frame of reference which solves for the conservation of mass, species, momentum and energy in the gas phase while using the Lagrangian frame of reference to obtain particle position, velocity and temperature of the feedstock. The particle-source-in cell approach was then used to couple the Eulerian and the Lagrangian frames. The particle dispersion was also solved by the stochastic model as shown in Fig. 2.

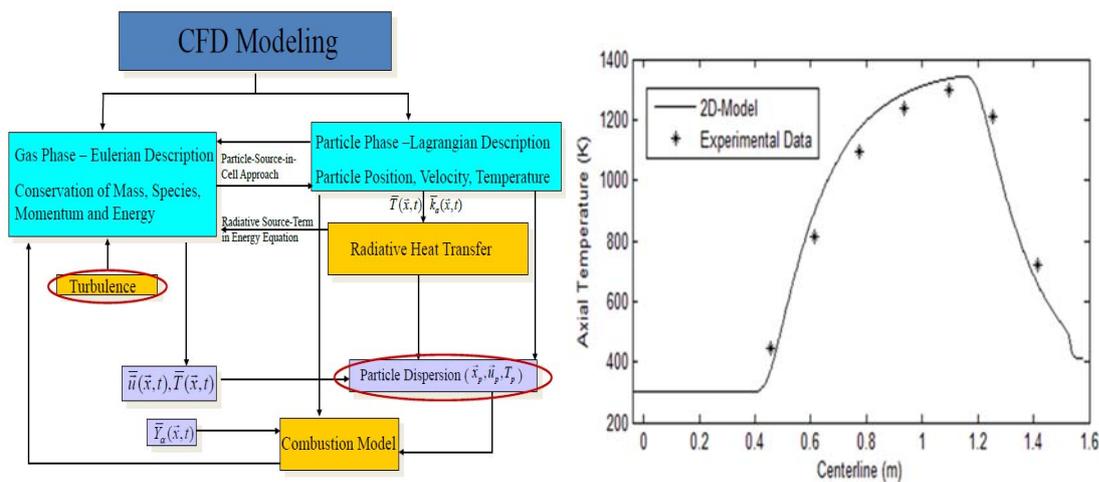


Fig. 2: Numerical solution approach for gasification [10] and axial temperature model validation

The validity of the results of every point on the contour depends mainly on the rigor of the constraint for the validation of the experimental data. The better the model results agree with the experimental values, the better fidelity of the model. Hence, the numerical model has been validated with experimental data obtained with the drop tube facilities at Masdar Institute. The model results predict the experimental values reasonably well as depicted in Fig. 3.

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