MASS TRANSFER SIMULATION OF A FLUIDIZED-BED GASIFIER USING PVC AS RAW MATERIAL

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Abstract. *Various alternative forms of energy generation have been researched as a consequence of the energetic crisis in global ambit. Particularly, energy generation from plastic wastes (PVC) via gasification process is a viable route. This gasification process is realized with the briquette plastic wastes and air or oxygen along with the steam in a fluidized bed gasifier/gas turbine (FBG/GT) system. In the present work, a model with only one chemical reaction taking part in the gasification process was considered. In this process, the components C,* CO_2*, CO,* H_2O *e* H_2 *resulting from gasification reactions are quantified as one system of partial differentials equations PDE's), thus, each component is represented for only one PDE. The solution of the system of PDE's was obtained by the implementation of one discretization scheme, which yields a system of algebraic equations (AE's). Then the system of AE's was solved by Newton Raphson's method.*

Keywords: *Gasification, PVC, Energy*

1. Introduction

Various alternative forms of energy generation have been researched as a consequence of the energetic crisis in global ambit. Solid waste, in dealing with the presence of organic compounds, especially plastics, can be considered an important source of alternative energy generation, since they are inexpensive and easily obtainable materials (Borgianni, 2001).

Gasification is an attractive thermochemical technology with higher efficiencies than combustion (Jong, 2003). Fluidized-bed reactors can be utilized in different thermal processes, like pyrolysis, gasification or combustion, aimed to energy or material recovery from solid wastes (Kaminsky, 1996). The fluidized bed has a number of special advantages for pyrolysis, because it is characterized by an excellent heat and mass transfer as well as a constant temperature throughout the reactor (Arena, 1999).

This gasification process is realized with the briquette plastic wastes (solid phase) and air or oxygen (ascendant gas phase) along with the steam in a fluidized bed gasifier/gas turbine (FBG/GT) system. In this process, the solid phase suffers partial oxidation and the resulting gasses are used in turbines. In the present work, a model with only one chemical reaction taking part in the gasification process was considered.

$$\frac{2(\alpha+\beta)}{(\alpha+2\beta)}C+O_2\rightarrow\frac{2\alpha}{(\alpha+2\beta)}CO+\frac{2\beta}{(\alpha+2\beta)}CO_2 \qquad (1)$$

Where α/β is the primary CO/CO_2 product ratio given by:

$$\alpha/\beta=A_1exp(-A_2/T_p) \qquad (2)$$

A_1 and A_2 are constants that may depend on the type of char, and T_p is the temperature of the particle (Chen et al, 2000).

The aim of this paper is obtain the concentration profiles from the components involved on the considerate reaction, using solid wastes containing PVC.

2. Mathematic model development:

The mathematic modeling using in this work was given in terms of compounds O_2, CO_2, CO and C. The modeling development is subordinate to the following simplifier hypothesis: (i) isothermal system, (ii) intraparticular diffusion effect isn't considered, (iii) models to compounds O_2, CO_2, CO and C are pseudo-heterogeneous with axial dispersion and (iv) constant gas density. According with this hypothesis, balance equations that describe the unsteady system behavior are given for a non-linear system of coupled partial differentials equations (PDE's), as shown below.

Mass Balance for O_2:

$$\frac{\partial(\varepsilon_g\rho_g Y_{O_2})}{\partial t}+\frac{Q_m}{A_s}\frac{\partial(\varepsilon_g\rho_g Y_{O_2})}{\partial z}=D_{O_2,eff}\frac{\partial^2(\varepsilon_g\rho_g Y_{O_2})}{\partial z^2}-R_{O_2} \tag{3}$$

Initial Conditions:

$$Y_{O_2}\big|_{t=0}=0{,}5 \tag{4}$$

Boundary Conditions:

$$DO_{2,eff}\frac{(\varepsilon_g\rho_g Y_{O_2})}{\partial z}\bigg|_{z=0^+}=\frac{Q_m}{A_S}[(\varepsilon_g\rho_g Y_{O_2})\big|_{z=0^+}-(\varepsilon_g\rho_g Y_{O_2})\big|_{z=0^-}] \tag{5}$$

$$\frac{\partial(\varepsilon_g\rho_g Y_{O_2})}{\partial z}\bigg|_{z=H}=0 \tag{6}$$

Mass Balance for CO_2:

$$\frac{\partial(\varepsilon_g\rho_g Y_{CO_2})}{\partial t}+\frac{Q_m}{A_s}\frac{\partial(\varepsilon_g\rho_g Y_{CO_2})}{\partial z}=D_{CO_2,eff}\frac{\partial^2(\varepsilon_g\rho_g Y_{CO_2})}{\partial z^2}+R_{CO_2} \tag{7}$$

Initial Conditions:

$$Y_{CO_2}\big|_{t=0}=0 \tag{8}$$

Boundary Conditions:

$$D_{CO_2,eff}\frac{\partial(\varepsilon_g\rho_g Y_{CO_2})}{\partial z}\bigg|_{z=0^+}=\frac{Q_m}{A_s}[(\varepsilon_g\rho_g Y_{CO_2})\big|_{z=0^+}-(\varepsilon_g\rho_g Y_{CO_2})\big|_{z=0^-}] \tag{9}$$

$$\frac{\partial(\varepsilon_g\rho_g Y_{CO_2})}{\partial z}\bigg|_{z=H}=0 \tag{10}$$

Mass Balance for CO:

$$\frac{\partial(\varepsilon_g\rho_g Y_{CO})}{\partial t}+\frac{Q_m}{A_s}\frac{\partial(\varepsilon_g\rho_g Y_{CO})}{\partial z}=D_{CO,eff}\frac{\partial^2(\varepsilon_g\rho_g Y_{CO})}{\partial z^2}+R_{CO} \tag{11}$$

Initial Conditions:

$$Y_{CO}\big|_{t=0}=0 \tag{12}$$

Boundary Conditions:

$$D_{CO,eff}\frac{\partial(\varepsilon_g\rho_g Y_{CO})}{\partial z}\Big|_{z=0^+} = \frac{Q_m}{A_s}[(\varepsilon_g\rho_g Y_{CO})\big|_{z=0^+} - (\varepsilon_g\rho_g Y_{CO})\big|_{z=0^-}] \qquad (13)$$

$$\frac{\partial(\varepsilon_g\rho_g Y_{CO})}{\partial z}\Big|_{z=H} = 0 \qquad (14)$$

Mass Balance For C:

$$\frac{\partial(\varepsilon_s\rho_s Y_C)}{\partial t} + \frac{F_s}{A_s}\frac{\partial(\varepsilon_s\rho_s Y_C)}{\partial z} = D_{C,eff}\frac{\partial^2(\varepsilon_s\rho_s Y_C)}{\partial z^2} - R_C \qquad (15)$$

Initial Conditions:

$$Y_C\big|_{t=0} = 0,5 \qquad (16)$$

Boundary Conditions:

$$D_{C,eff}\frac{\partial(\varepsilon_s\rho_s Y_C)}{\partial z}\Big|_{z=0^+} = \frac{F_s}{A_s}[(\varepsilon_s\rho_s Y_C)\big|_{z=0^+} - (\varepsilon_s\rho_s Y_C)\big|_{z=0^-}] \quad \frac{\partial(\varepsilon_s\rho_s Y_C)}{\partial z}\Big|_{z=H} = 0 \qquad (17)$$

3. Kinetics modeling

The Corresponding rate to equation 1 is given in the bellow table:

Table 1: Reaction kinetic rates

Reaction Rate	Reference
$R_1 = K_1 C_{O_2}$; $K_1 = 250T_p exp\left(\frac{-19000}{T_p}\right)F_p$	Chen at al (2000)

Where F_p is the specific internal surface area of the char (Chen at al 2000).

The total consumption and formation rates, R_i, for each component can be obtained using the equation follow (Xiu et al, 2002):

$$R_i = \sum_{j=1}^{2} \nu_{ij} R_j \qquad (18)$$

Where, ν_{ij} is the stoichiometric coefficient of compound i in the j reaction. If ν_{ij} refers to reactants, ν_{ij} is negative, and for a product ν_{ij} is positive. In this way, the total rate for each compound is given to:

$$R_{O2} = -R_1 \qquad (19)$$

$$R_{CO2} = +\left(\frac{2\beta}{\alpha + 2\beta}\right)R_1 - R_2 \qquad (20)$$

$$R_{CO}=+\left(\frac{2\alpha}{\alpha+\beta}\right)R_1+\frac{1}{2}R_2 \tag{21}$$

4. Numerical methodology

The equations, with the total consumption and formation rates yield a non-linear system of coupled partial differentials equations (PDE's), an initial value and boundary problem. These equations are too complex for analytical solving. Then the Explicit Euler (EE) method was used as predictor and Implicit Euler (IE) method as corrector to solve the PDE's system. This system was solved using spatial derivatives discretization by finite differences and the resulting system of ordinary differential equations (ODE's) by Euler's Method.

Discretized Mass Balance for O_2:

$$\frac{d(Y_{O_2})}{dt}=\frac{D_{O_{2,eff}}}{\Delta z^2}\left[(Y_{O_2})_{i+1}-2(Y_{O_2})_i+(Y_{O_2})_{i-1}\right]-\frac{Q_m}{A_s\Delta z}\left[(Y_{O_2})_{i+1}-(Y_{O_2})_i\right]-R_{O_2} \tag{22}$$

Discretized Boundary and Initial Conditions:

$$(Y_{O_2})_{i-1}=0{,}5 \tag{23}$$

$$(Y_{O_2})_{i+1}=-\frac{D_{O_{2,eff}}+U\Delta z(Y_{O_2})_i-2U\Delta z(Y_{O_2})_{i-1}}{-D_{O_{2,eff}}+U\Delta z} \tag{24}$$

$$(Y_{O_2})_{N-1}=(Y_{O_2})_N \tag{21}$$

Discretized Mass Balance for CO_2:

$$\frac{d(Y_{CO_2})}{dt}=\frac{D_{CO_{2,eff}}}{\Delta z^2}\left[Y_{CO_{2\,i+1}}-2Y_{CO_{2\,i}}+Y_{CO_{2\,i-1}}\right]-\frac{Q_m}{A_s\Delta z}\left[Y_{CO_{2\,i+1}}-Y_{CO_{2\,i}}\right]+R_{CO_2} \tag{25}$$

Discretized Boundary and Initial Conditions:

$$(Y_{CO_2})_{i-1}=0 \tag{26}$$

$$(Y_{CO_2})_{i+1}=-\frac{D_{CO_{2,eff}}+U\Delta z(Y_{CO_2})_i-2U\Delta z(Y_{CO_2})_{i-1}}{-D_{CO_{2,eff}}+U\Delta z} \tag{27}$$

$$(Y_{CO_2})_{N-1}=(Y_{CO_2})_N \tag{28}$$

Discretized Mass Balance for CO:

$$\frac{d(Y_{CO})}{dt}=\frac{D_{CO_{,eff}}}{\Delta z^2}\left[Y_{CO\,i+1}-2Y_{CO\,i}+Y_{CO\,i-1}\right]-\frac{Q_m}{A_s\Delta z}\left[Y_{CO\,i+1}-Y_{CO\,i}\right]+R_{CO} \tag{29}$$

Discretized Boundary and Initial Conditions:

$$(Y_{CO})_{i-1}=0 \tag{30}$$

$$(Y_{CO})_{i+1}=-\frac{D_{CO_{,eff}}+U\Delta z(Y_{CO})_i-2U\Delta z(Y_{CO})_{i-1}}{-D_{CO_{,eff}}+U\Delta z} \tag{31}$$

$$(Y_{CO})_{N-1}=(Y_{CO})_N \tag{32}$$

Discretized Mass Balance for C:

$$\frac{d(Y_C)}{dt}=\frac{D_{C,eff}}{\Delta z^2}\left[(Y_C)_{i+1}-2(Y_C)_i+(Y_C)_{i-1}\right]-\frac{F_s}{A_s\Delta z}\left[(Y_C)_{i+1}-(Y_C)_i\right]-R_C \tag{33}$$

Discretized Boundary and Initial Conditions:

$$(Y_C)_{i-1}=1 \tag{34}$$

$$(Y_C)_{i+1}=-\frac{D_{C,eff}(Y_C)_i-2U\Delta z(Y_C)_{i-1}}{-D_{C,eff}+U\Delta z} \tag{35}$$

$$(Y_C)_{N-1}=(Y_C)_N \tag{36}$$

5. Discussion and results

In this section, results from the model predictions are presented. Simulations were performed in order to determine the emissions of CO_2 and CO from the fluidized bed reactor. To realize the simulation, some complementary parameters are used. This parameters are given in the Table 2.

Table 2. Complementary parameters simulation

Parameters	Values
A_1	750
A_2	7200
T_p	700

Figure 1 demonstrate the unsteady profile of carbon consumption reveling a high reactor rate associated with combustion nature.

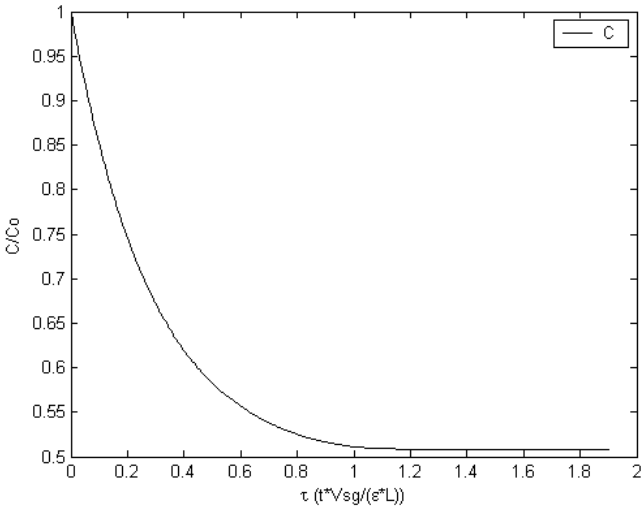

Figure 1. Unsteady profile of carbon consumption

Figures 2 and 4 demosntrate the unsteady profile of O_2 and CO molar fraction at the end of reactor, respctively. Since CO molar fraction is too small was necessary a isolated graphic to demonstrate its profile.

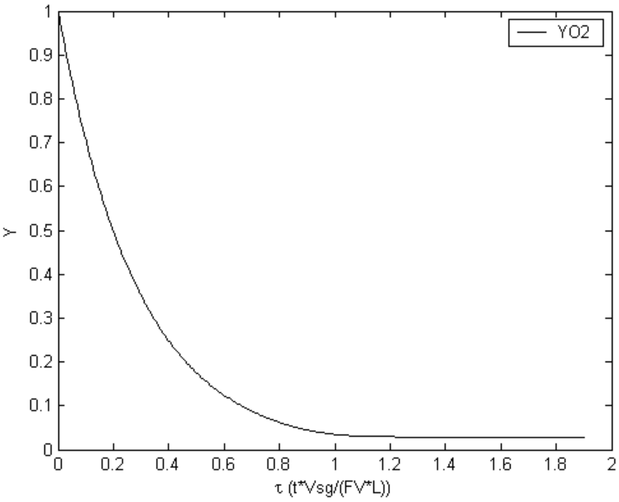

Figure 2. Unsteady profile of O_2 molar fraction

Figure 3 demonstrate all gaseous phase fractions profile at the end of reactor. Note the small CO molar fraction.

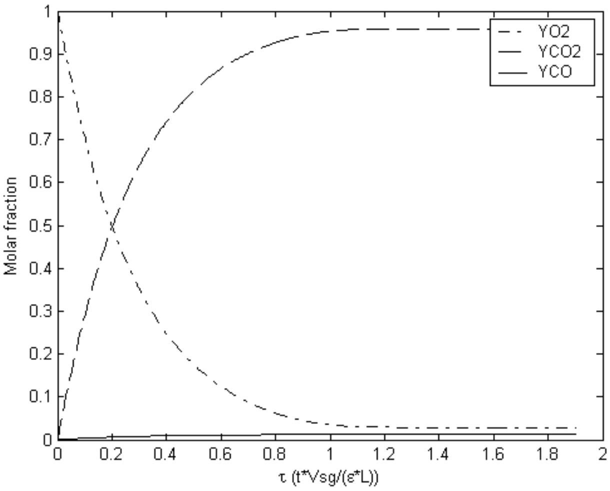

Figure 3. Unsteady profiles of gaseous fractions at z = L

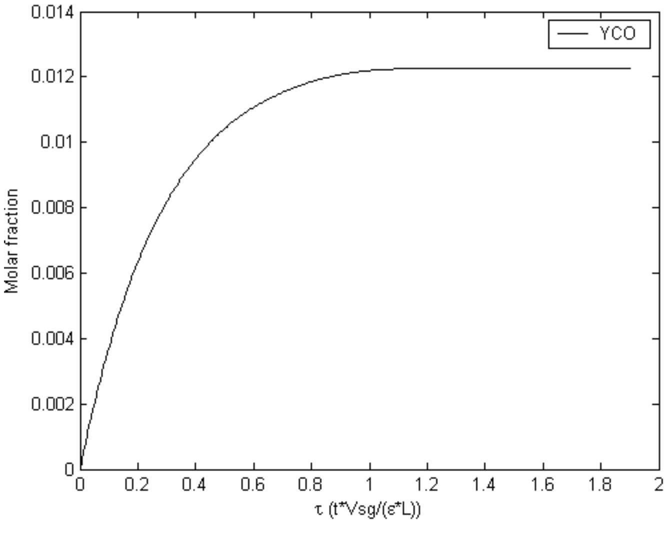

Figure 4. Unsteady profile of CO molar fraction at z=L

Figures 5 and 6 demonstrate the overall Unsteady profile of O_2 and CO molar fraction over reactor length.

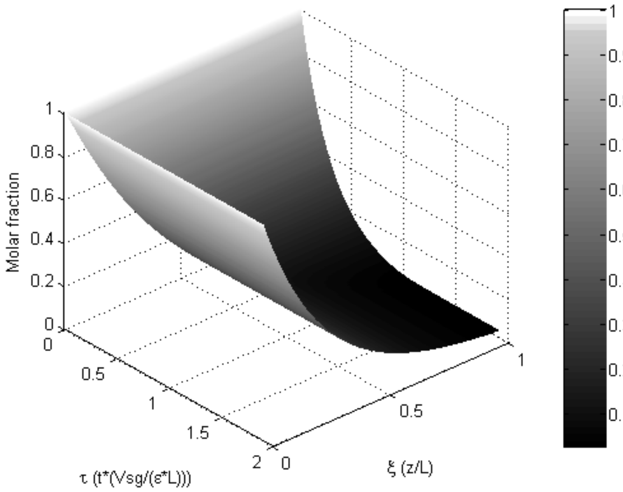

Figure 5. Unsteady profile of O_2 molar fraction over reactor length

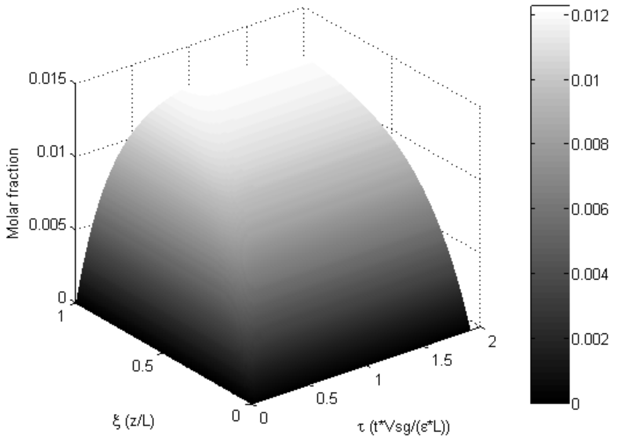

Figure 6. Unsteady profile of CO over reactor length

6. Conclusions

The behavior of components C, O_2 and CO was obtained in this work. For this, the modeling for each component was developed and then the simulation of the model was carried out for the established conditions. By taking this in consideration, we can take the following conclusions:

- The relative concentration of C decays over time, reaching stationary state at $\tau = 1,6$.
- O_2 reaches stationary state at $\tau = 1,4$.
- At the end of the reactor ($x = L$), CO_2 molar fraction grows up until get stabilized at $\tau = 1,4$.
- There is a small variation of CO molar fraction. In fact, it increases slightly until get stabilized at $\tau = 1,1$.

So, it can be concluded that, for the purposes of CO production and at these conditions, the reaction took place in a small interval and had little efficiency.

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8. Notations

F_p	Specified area, m^{-1}
R	Gas universal constant, m^3 Pa/mol K
t	Temporal coordinates, s
z	Spatial coordinates, m
T_p	Temperature of the particle, K
$D_{i,eff}$	Effective diffusivity of compound, i= O_2, CO_2
d_s	Solid-phase diameter, m
L	FB height, m
P	Pressure, Pa
$Q_{ar,0}$	Inlet gas-phase inlet out flow, m^3/s
Q_{ar}	Gas-phase inlet out flow, m^3/s
Vs_g	Gas superficial velocity, m/s
Y_i	Gaseous compounds molar fraction, i= O_2, CO_2
Y_C	Carbon molar fraction

9. Greeks letters

ε_g	Gas-phase void fraction
ε_s	Solid-phase void fraction
ρ_g	Gas-phase (air) density, kg/m^3
τ	Dimensionless time
ξ	Dimensionless space
ρ_s	Solid-phase (solid wastes) density, kg/m^3

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