

## MASS TRANSFER SIMULATION OF A FLUIDIZED-BED GASIFIER USING SUGAR CANE BAGASSE AS FUEL

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**Abstract.** *Fluidized-bed gasifiers technology has been developed in order to achieve solid fuel conversion to electric energy. In this case, the fuel considered is cane sugar bagasse. Mathematical modelling was developed by taking in account the axial dispersion, convection and reaction effects in the reactor. The model is one dimensional. Danckwerts boundary conditions were applied. This set of partial differential equations is then discretized and then we obtain a set of algebraic equations which is solved to give the concentration of components and the temperature profiles of the solid and gaseous phase.*

**Keywords:** *Gasification, fluidized-bed, partial oxidation*

## 1. Introduction

The interest in use of renewable energy sources, e.g. biomass and municipal solid waste as fuels is expected to increase in the future because of the need to reduce the net CO<sub>2</sub> emission (Zhou, 2004). Also, crisis in Brazilian electric energy supply system has forced its government to improve investments in alternative sources looking for a quantitative increase in national production.

Biomass, biodiesel and aeolic energy are concrete examples of this new behavior. But national biomass gasification coupled with thermoelectric systems technology is still in early development, compared with other countries. According to a recent survey, there are nearly 100 biomass gasification and/or pyrolysis installations in Europe and North America (Li, 2003). The implementation of such a industrial-scale plant could bring benefits to traditional sugar-cane planters, like Brazilian Northeast. It also could reduce the pollutants emission.

Biomass gasification produces fuel gas or synthesis gas through the chemical conversion of biomass, usually involving partial oxidation of the feedstock in a reducing atmosphere in the presence of air, oxygen and/or steam (Li, 2003). A typical system would be a fluidized-bed reactor with a gaseous phase (air or steam) and an ascending solids phase (in this case, sugar cane briquettes) which undergoes a partial oxidation, the gaseous products being used in a turbine. Along with this gaseous products are CO, O<sub>2</sub>, H<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>O and N<sub>2</sub>.

Since it's necessary to run a partial oxidation as the key point of the process, it also become of very difficult control. Follows that is necessary to develop an adequate methodology for plant behavior prediction. For this reason, one of the first steps of the development of such a technology evolves the adoption of a consistent mathematical model, which describes with reasonable precision what's happening on process. Several different types of models have been developed for gasification systems—kinetic, equilibrium, and others. In this work, a model with two chemical reactions, as taking part in the gasification process was considered:



Where  $\alpha/\beta$  is the primary CO/CO<sub>2</sub> product ratio given by:

$$\alpha/\beta = A_1 \exp(-A_2/T_p) \quad (3)$$

$A_1$  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 objective of this study is to provide a theoretical perspective for scale-up from mathematical modeling.

## 2. Mathematic model development:

The mathematic modeling using in this work was given in terms of compounds O<sub>2</sub>, CO<sub>2</sub>, CO and C. The modeling development is subordinate to the following simplifier hypothesis: (i) isothermal system, (ii) intraparticle diffusion effect isn't considered, (iii) models to compounds O<sub>2</sub>, CO<sub>2</sub>, 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<sub>2</sub>:

$$\frac{\partial(\epsilon_g \rho_g Y_{O_2})}{\partial t} + \frac{Q_m}{A_s} \frac{\partial(\epsilon_g \rho_g Y_{O_2})}{\partial z} = D_{O_2, eff} \frac{\partial^2(\epsilon_g \rho_g Y_{O_2})}{\partial z^2} - R_{O_2} \quad (4)$$

Initial Conditions:

$$Y_{O_2}|_{t=0} = I \quad (5)$$

Boundary Conditions:

$$D_{O_2, eff} \frac{\partial(\epsilon_g \rho_g Y_{O_2})}{\partial z} \Big|_{z=0^+} = \frac{Q_m}{A_s} [(\epsilon_g \rho_g Y_{O_2}) \Big|_{z=0^+} - (\epsilon_g \rho_g Y_{O_2}) \Big|_{z=0^-}] \quad (6)$$

$$\frac{\partial(\epsilon_g \rho_g Y_{O_2})}{\partial z} \Big|_{z=H} = 0 \quad (7)$$

Mass Balance for CO<sub>2</sub>:

$$\frac{\partial(\epsilon_g \rho_g Y_{CO_2})}{\partial t} + \frac{Q_m}{A_s} \frac{\partial(\epsilon_g \rho_g Y_{CO_2})}{\partial z} = D_{CO_2, eff} \frac{\partial^2(\epsilon_g \rho_g Y_{CO_2})}{\partial z^2} + R_{CO_2} \quad (8)$$

Initial Conditions:

$$Y_{CO_2}|_{t=0} = 0 \quad (9)$$

Boundary Conditions:

$$D_{CO_2, eff} \frac{\partial(\epsilon_g \rho_g Y_{CO_2})}{\partial z} \Big|_{z=0^+} = \frac{Q_m}{A_s} [(\epsilon_g \rho_g Y_{CO_2}) \Big|_{z=0^+} - (\epsilon_g \rho_g Y_{CO_2}) \Big|_{z=0^-}] \quad (10)$$

$$\frac{\partial(\epsilon_g \rho_g Y_{CO_2})}{\partial z} \Big|_{z=H} = 0 \quad (11)$$

Mass Balance for CO:

$$\frac{\partial(\epsilon_g \rho_g Y_{CO})}{\partial t} + \frac{Q_m}{A_s} \frac{\partial(\epsilon_g \rho_g Y_{CO})}{\partial z} = D_{CO, eff} \frac{\partial^2(\epsilon_g \rho_g Y_{CO})}{\partial z^2} + R_{CO} \quad (12)$$

Initial Conditions:

$$Y_{CO}|_{t=0} = 0 \quad (13)$$

Boundary Conditions:

$$D_{CO,eff} \frac{\partial(\varepsilon_g \rho_g Y_{CO})}{\partial z} \Big|_{z=0^+} = \frac{Q_m}{A_s} [(\varepsilon_g \rho_g Y_{CO}) \Big|_{z=0^+} - (\varepsilon_g \rho_g Y_{CO}) \Big|_{z=0^-}] \quad (14)$$

$$\frac{\partial(\varepsilon_g \rho_g Y_{CO})}{\partial z} \Big|_{z=H} = 0 \quad (15)$$

Mass Balance For C:

$$\frac{\partial(\varepsilon_s \rho_s Y_C)}{\partial t} + \frac{F_s}{A_s} \frac{\partial(\varepsilon_s \rho_s Y_C)}{\partial z} = D_{C,eff} \frac{\partial^2(\varepsilon_s \rho_s Y_C)}{\partial z^2} - R_C \quad (16)$$

Initial Conditions:

$$Y_C|_{t=0} = 0,5 \quad (17)$$

Boundary Conditions:

$$D_{C,eff} \frac{\partial(\varepsilon_s \rho_s Y_C)}{\partial z} \Big|_{z=0^+} = \frac{F_s}{A_s} [(\varepsilon_s \rho_s Y_C) \Big|_{z=0^+} - (\varepsilon_s \rho_s Y_C) \Big|_{z=0^-}] \quad \frac{\partial(\varepsilon_s \rho_s Y_C)}{\partial z} \Big|_{z=H} = 0 \quad (18)$$

### 3. Kinetics modeling

The Corresponding rate to equation 1 and 2 are given in the Table 1:

Table 1: Reaction kinetic rates

Reaction Rate	Reference
$R_1 = K_1 C_{O_2}; K_1 = 250 T_p \exp\left(\frac{-19000}{T_p}\right) F_p$	Chen at al (2000)
$R_2 = K_2 C_{CO_2}; K_2 = 4364 \exp\left(\frac{-29884}{T_p}\right) F_p$	

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):

$$R_i = \sum_{j=1}^2 v_{ij} R_j \quad (19)$$

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

$$R_{O_2} = -R_I \quad (20)$$

$$R_{CO_2} = + \left( \frac{2\beta}{\alpha + 2\beta} \right) R_I - R_2 \quad (21)$$

$$R_{CO} = + \left( \frac{2\alpha}{\alpha + \beta} \right) R_I + \frac{1}{2} R_2 \quad (22)$$

#### 4. Numerical methodology

The equations, with the total consumption and formation rates yield a non-linear system of coupled partial differential 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<sub>2</sub>:

$$\frac{d(Y_{O_2})}{dt} = \frac{D_{O_2,eff}}{\Delta z^2} [Y_{O_2,i+1} - 2(Y_{O_2})_i + (Y_{O_2})_{i-1}] - \frac{Q_m}{A_s \Delta z} [Y_{O_2,i+1} - (Y_{O_2})_i] - R_{O_2} \quad (23)$$

Discretized Boundary and Initial Conditions:

$$(Y_{O_2})_{i-1} = 0,5 \quad (24)$$

$$(Y_{O_2})_{i+1} = - \frac{D_{O_2,eff} + U\Delta z(Y_{O_2})_i - 2U\Delta z(Y_{O_2})_{i-1}}{-D_{O_2,eff} + U\Delta z} \quad (25)$$

$$(Y_{O_2})_{N-1} = (Y_{O_2})_N \quad (26)$$

Discretized Mass Balance for CO<sub>2</sub>:

$$\frac{d(Y_{CO_2})}{dt} = \frac{D_{CO_2,eff}}{\Delta z^2} [Y_{CO_2,i+1} - 2Y_{CO_2,i} + Y_{CO_2,i-1}] - \frac{Q_m}{A_s \Delta z} [Y_{CO_2,i+1} - Y_{CO_2,i}] + R_{CO_2} \quad (27)$$

Discretized Boundary and Initial Conditions:

$$(Y_{CO_2})_{i-1} = 0 \quad (28)$$

$$(Y_{CO_2})_{i+1} = - \frac{D_{CO_2,eff} + U\Delta z(Y_{CO_2})_i - 2U\Delta z(Y_{CO_2})_{i-1}}{-D_{CO_2,eff} + U\Delta z} \quad (29)$$

$$(Y_{CO_2})_{N-1} = (Y_{CO_2})_N \quad (30)$$

Discretized Mass Balance for CO:

$$\frac{d(Y_{CO})}{dt} = \frac{D_{CO,eff}}{\Delta z^2} [Y_{CO,i+1} - 2Y_{CO,i} + Y_{CO,i-1}] - \frac{Q_m}{A_s \Delta z} [Y_{CO,i+1} - Y_{CO,i}] + R_{CO} \quad (31)$$

Discretized Boundary and Initial Conditions:

$$(Y_{CO})_{i-1} = 0 \quad (32)$$

$$(Y_{CO})_{i+1} = -\frac{D_{CO,eff} + U\Delta z(Y_{CO})_i - 2U\Delta z(Y_{CO})_{i-1}}{-D_{CO,eff} + U\Delta z} \quad (33)$$

$$(Y_{CO})_{N-1} = (Y_{CO})_N \quad (34)$$

Discretized Mass Balance for C:

$$\frac{d(Y_C)}{dt} = \frac{D_{C,eff}}{\Delta z^2}[(Y_C)_{i+1} - 2(Y_C)_i + (Y_C)_{i-1}] - \frac{F_s}{A_s \Delta z}[(Y_C)_{i+1} - (Y_C)_i] - R_C \quad (35)$$

Discretized Boundary and Initial Conditions:

$$(Y_C)_{i-1} = 1 \quad (36)$$

$$(Y_C)_{i+1} = -\frac{D_{C,eff}(Y_C)_i - 2U\Delta z(Y_C)_{i-1}}{-D_{C,eff} + U\Delta z} \quad (37)$$

$$(Y_C)_{N-1} = (Y_C)_N \quad (38)$$

## 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<sub>2</sub> and CO from the fluidized bed reactor. To realize the simulation, some complementary parameters are used. This parameters are given in the Table 2.

Figure 1 shows the profile of CO molar fraction over time, since it's a desirable product. At the temperature used in this work, we achieve a small production of that component.

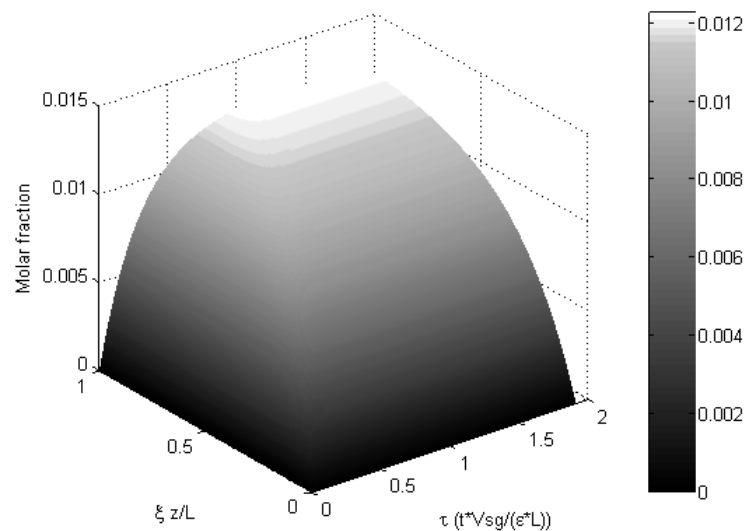


Figure 1. Unsteady profile of CO molar fraction over reactor length

Figure 2 and 3 show the unsteady profiles over the reactor length for O<sub>2</sub> and CO<sub>2</sub>, respectively. The high production of CO<sub>2</sub> reflects the necessity of post processing of residues of combustion in order to diminish the pollutant emissions.

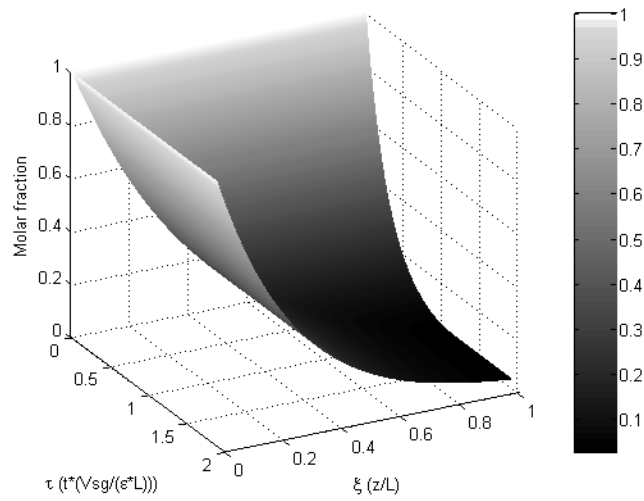


Figure 2. Unsteady profile of  $O_2$  molar fraction over reactor length

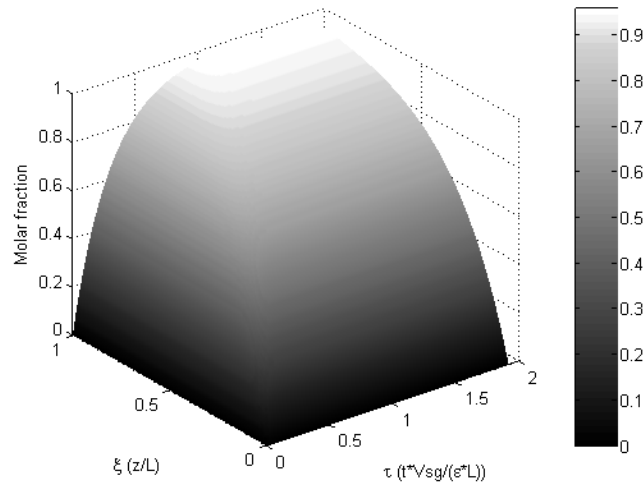


Figure 3. Unsteady profile of  $CO_2$  molar fraction over reactor length

Figure 4 shows the overall gas composition at the end of the reactor, i.e., at  $z=L$ . It can be observed that CO production is very small in comparison with the other components.

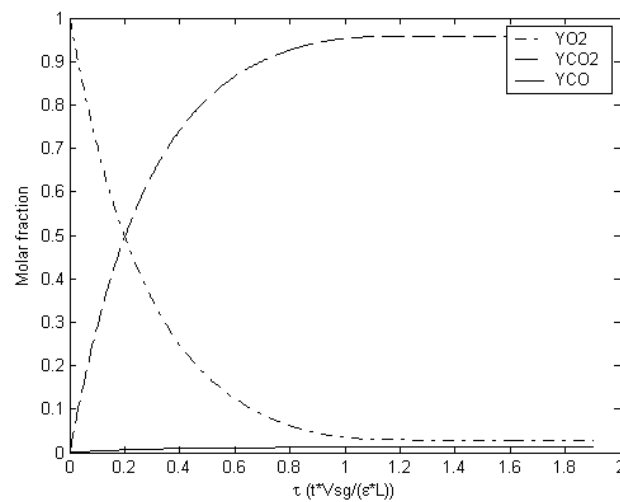


Figure 4. Unsteady profiles of gaseous fractions at  $z = L$

The equilibrium is achieved very early, reflecting the high velocity of combustion. Also, in Figure 5 it is shown the profile of char consumption over time.

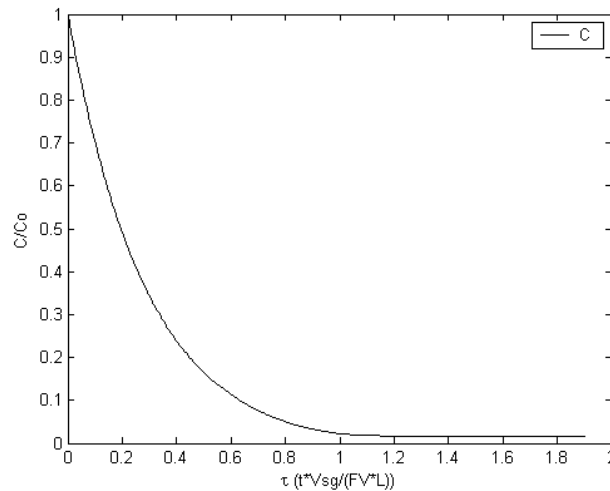


Figure 5. Unsteady profile of carbon consumption at  $z=L$

Table 2. Complementary parameters simulation

Parameters	Values
$A_1$	750
$A_2$	7200
$T_p$	700

## 6. Conclusion and future work

The profiles of gaseous components and of char consumption were calculated at a given temperature. Production of CO is too small at these conditions. The calculated results strongly depends on the parameters  $A_1$  and  $A_2$ , which are lacking for the specific case of sugar cane bagasse. These parameters could be obtained in laboratory. Future work may include the determination of them and couple mass and energy balances over the reactor in order to achieve more accurate profiles, since they will reflect the reactor behavior as the temperature rises.

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## 8. Notations

- $F_p$  Specific 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,  $m^3/s$
- $V_{sg}$  Gas superficial velocity, m/s
- $Y_i$  Gaseous compounds molar fraction,  $i= O_2, CO_2$
- $Y_C$  Carbon molar fraction

## 9. Greeks letters

- $\varepsilon_g$  Gas-phase void fraction  
 $\varepsilon_s$  Solid-phase void fraction  
 $\rho_g$  Gas-phase (air) density,  $\text{kg/m}^3$   
 $\tau$  Dimensionless time  
 $\xi$  Dimensionless space  
 $\rho_s$  Solid-phase (solid wastes) density,  $\text{kg/m}^3$

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