DYNAMIC ANALYSIS OF THE THERMAL AND MASS EFFECTS OF A FLUIDIZED BED GASIFIER GASIFICATION REGION

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Abstract. The combustible gases production such as CO and H_2 derived from a biomass, achieved notoriety in the worldwide energy matrix. Nowadays, these gases are used to generate electricity in fluidized bed gasification systems. The process of biomass gasification in a fluidized bed can be divided into three main zones: combustion, reduction and freeboard. In the combustion zone, the biomass reacts with the hot air flow which enters roughly through a distributor. In this zone, the system reaches between 900°C-1430°C, releasing energy into the reduction region due to the combustion reaction. In the presented work, the study was restricted to mathematical modelling in order to analyze, not only the thermal, but also the mass effects in the combustion region. The mathematical model developed to use in the combustion zone, formed by the partial differential equations system, was converted into a system of ODE and then the Ruge Kutta Gill method was put into practice. This way, thermal as well as mass effects were analyzed in the combustion region. Moreover, the production of CO and H_2 as well as a sensitive analysis, were examined so as to validate the parameters which influence the dynamic model developed.

Keywords: Gasifier, fluidized-bed, energy, biomass, solid fuel.

1. INTRODUCTION

The politic strategies of the Brazilian electric sector foresee an amplification of the electric energy production from renewable sources. However, the electric energy production from the gasification of solid biomass wastes is a promising alternative technology for this sector. This technology involves an integration process, fluidized-bed gasifier (FBG)/gas turbine (GT), which can be configured by a simple integration, that is, hardly a GT integrated to FBG or through combined cycle (Brayton/Rankine) that includes the integration of a GT and a steam turbine (ST) integrated to FBG (Gabra et al., 2001a, b, c).

The biomass gasification technology in a FBG needs the detailed knowledge of the physical and chemical phenomenon to optimize the energy efficiency in the gasifier. However, the mathematical models are important tools to investigate these physical and chemical phenomenons that happen in the FBG. The mathematical models are usually composed by moment, energy and mass balance equations. In the present work, it was just studied the energy and mass balance equations.

The FBG for a simple cycle plant or for a combined cycle plant is an equipment with complex operation. Therefore, the gasification reactions of operational control are difficult tasks. The referring mass balance equations to each component (reagents and products) of the gasification process compose the mathematical modelling for the FBG. The mathematical modelling developed for the FBG was used to simulate the gasification reactions components behavior, as well as the thermal behavior in the FBG.

The energy and mass balance equations developed for the gasification process form a coupled partial differential equation (PDEs) system. The numerical solution of this PDEs system was accomplished with implementation of Runge-Kutta Gill method (Silva et al, 2002a, 2004b).

The cane bagasse is a promising solid fuel for the power generation system in FBG with high efficiency and at low cost (Gabra et al., 2001, Bridgewater, 1995). Before the gasification process to be accomplished, the cane bagasse suffers a pre-treatment as the following steps: (i) the cane bagasse is briquetted; (ii) drying to evaporate moisture; (iii) it should be heated up to 300°C-500°C.

The gasification process involves the solid fuel entrance in the top of the FBG and the air and steam entrance in the base of the FBG. In the gasification zone happens homogeneous and heterogeneous reactions.

$C + O_2 \Leftrightarrow CO_2$	(I)
$C + H_2O \Leftrightarrow CO + H_2$	(II)
$\rm CO + H_2O \Leftrightarrow \rm CO_2 + H_2$	(III)
$C + CO_2 \Leftrightarrow 2 CO$	(IV)
Therefore the chieving of this much is to exclude the components habening resulting (C. CO. O. H. CO.	II O

Therefore, the objective of this work is to analyze the components behavior resulting (C, CO, O_2 , H_2 , CO_2 , H_2O) of the gasification process through the modelling and simulation.

2. THE PHYSICAL MODELLING DEVELOPMENT FOR THE GASIFICATION PROCESS

Fluidized-bed gasifier (FBG) is usually divided in two zones: (i) a fluid-solid fluidization zone; (ii) a solid free zone (Freeboard). The mathematical modelling developed for this work was just restricted to fluid-solid fluidization zone. In this zone will happen the combustion and gasification' reactions. The Figure 1 shows the FBG simplified prototype that will be used for the simulation of this work.



Figure 1. A fluidized-bed gasifier simplified model (FBG) for the electric energy production

In Figure 1, it was shown a FBG prototype, it is used as tool to accomplish the numeric experiments presented in the present work for the gasification process. The mathematical model developed for this work was formulated with relation to temperatures of the gaseous and solid phases with relation to components O_2 , CO, CO_2 , H_2O , H_2 and C. This modelling development is subjecting the following simplifying hypotheses: (i) nonisothermal system with energy balance for the gaseous and solid phases one-dimensional; (ii) temperatures of the gaseous and solid phases are modelled as models of thermal axial dispersion; (iii) the mathematical models for the components O_2 , CO, CO_2 , H_2O ,

Energy balance for the gaseous phase;

$$\varepsilon_{g} \rho_{g} C_{p,g} \frac{\partial T_{g}}{\partial t} + \frac{\varepsilon_{g} \rho_{g} C_{p,g} Q_{g}}{A_{s}} \frac{\partial T_{g}}{\partial z} = \varepsilon_{g} \lambda_{g,eff} \frac{\partial^{2} T_{g}}{\partial z^{2}} - \varepsilon_{s} h_{gs} (T_{g} - T_{S}) + (-\Delta H_{r,3}) R_{3,homog}$$
(1)

Initial and boundary conditions;

$$\left. T_{g} \right|_{t=0} = 0 \tag{2}$$

$$\lambda_{g,eff} \frac{\partial T_g}{\partial z} \bigg|_{z=0^+} = \frac{\rho_g C_{p,g} Q_g}{A_S} \bigg[T_g \bigg|_{z=0^+} - T_g \bigg|_{z=0^-} \bigg]$$
(3)

$$\frac{\partial T_g}{\partial z} \bigg|_{z = H} = 0$$
⁽⁴⁾

• Energy balance for the solid phase;

$$\varepsilon_{s}\rho_{s}C_{p,s}\frac{\partial T_{s}}{\partial t} + \frac{\varepsilon_{s}\rho_{s}C_{p,s}F_{s}}{A_{s}}\frac{\partial T_{s}}{\partial z} = \varepsilon_{s}\lambda_{s,eff}\frac{\partial^{2}T_{s}}{\partial z^{2}} + \varepsilon_{s}h_{gs}\left(T_{s} - T_{g}\right) + \rho_{s}\sum_{j=1}^{3}\eta_{e,j}R_{j}\left(-\Delta H_{j}\right)$$
(5)

• Initial and boundary conditions;

$$T_{s}\big|_{t=0} = 0 \tag{6}$$

$$\lambda_{s, eff} \frac{\partial T_{s}}{\partial z} \bigg|_{z=0^{+}} = \frac{\rho_{s} C_{p,s} F_{s}}{A_{s}} \Big[T_{s} \big|_{z=0^{+}} - T_{s} \big|_{z=0^{-}} \Big]$$

$$\frac{\partial T_{s}}{\partial z} \bigg|_{z=0^{+}} = 0$$
(8)

$$\frac{\partial z}{\partial z}\Big|_{z = H} = 0$$
(8)

• Balances for the gaseous species O_2 , CO, CO_2 , H_2O and H_2 .

$$\frac{\partial \left(\epsilon_{g} \rho_{g} Y_{i}\right)}{\partial t} + \frac{Q_{g}}{A_{s}} \frac{\partial \left(\epsilon_{g} \rho_{g} Y_{i}\right)}{\partial z} = D_{i, eff} \frac{\partial^{2} \left(\epsilon_{g} \rho_{g} Y_{i}\right)}{\partial z^{2}} + \frac{R T_{g}}{P} R_{i}; i=O_{2}, CO, CO_{2}, H_{2}O \text{ and } H_{2}$$
(9)

• Initial and boundary conditions;

$$Y_i \Big|_{t=0} = 0 \tag{10}$$

$$D_{i,eff} \frac{\partial \left(\varepsilon_{g} \rho_{g} Y_{i}\right)}{\partial z} \bigg|_{z=0^{+}} = \frac{Q_{g}}{A_{S}} \bigg[\left(\varepsilon_{g} \rho_{g} Y_{i}\right) \bigg|_{z=0^{+}} - \left(\varepsilon_{g} \rho_{g} Y_{i}\right) \bigg|_{z=0^{-}} \bigg]$$
(11)

$$\frac{\partial \left(\varepsilon_{g} \rho_{g} Y_{i}\right)}{\partial z} \bigg|_{z = H} = 0$$
(12)

The C that appears in the heterogeneous chemical reactions is given in function of the burns rate of the individual C particles (Basu, 1999).

$$\frac{\partial(\epsilon_{\rm s}\,\rho_{\rm s}\,Y_{\rm C})}{\partial t} + \frac{F_{\rm s}}{A_{\rm s}}\frac{\partial(\epsilon_{\rm s}\,\rho_{\rm s}\,Y_{\rm C})}{\partial z} = D_{\rm C,\,eff}\frac{\partial^2(\epsilon_{\rm g}\,\rho_{\rm g}\,Y_{\rm C})}{\partial z^2} - 3\frac{R\,T_{\rm g}}{P}R_{\rm C}$$
(13)

• Initial and boundary conditions;

$$Y_{C}\Big|_{t=0} = 0 \tag{14}$$

$$D_{C,eff} \frac{\partial \left[\epsilon_g \rho_g Y_C \right]}{\partial z} \bigg|_{z=0^+} = \frac{F_s}{A_S} \left[\left[\left[\epsilon_g \rho_g Y_C \right]_{z=0^+} - \left[\epsilon_g \rho_g Y_C \right]_{z=0^-} \right] \right]$$
(15)

$$\frac{\partial \left(\varepsilon_{g} \rho_{g} Y_{C} \right)}{\partial z} \bigg|_{z = H} = 0$$
(16)

3. MATHEMATICAL MODELLING FOR THE KINETICS

The chemical equation system presented by the I to IV reactions couples one homogeneous reaction and three heterogeneous reactions. The reactions I, II and IV were classified as heterogeneous reactions, while the III reaction was classified as homogeneous. In the Table 1, the corresponding rates for each one of these reactions were presented:

Table 1.	Kinetic	rates for	I, II,	III and	IV	reactions,	References.
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Reactions Rates	References
$R_{I} = 6.0 \times 10^{7} \left(\frac{Y_{O_{2}}}{2}\right) exp\left(-\frac{29.790}{T_{s}}\right)$	Calleja et al (1981)
$R_{II} = 14.4 \text{ S exp}\left(\frac{-166156}{\text{RT}}\right) C_{\text{H}_2\text{O}}^{0,83} (1000)^{-0.17} \varepsilon_c$	Jong <i>et al</i> (2003)
$R_{III} = 1.3 \times 10^{11} \phi \left(\frac{RT_g}{P}\right)^{1/2} \left(\frac{Y_{O_2}}{2}\right)^{1/2} exp\left(-\frac{15098}{T_s}\right)^{1/2}$	Ross e Davidson (1982)
$R_{I} = 3.0 \times 10^{5} \left(\frac{Y_{O_{2}}}{2}\right) exp\left(-\frac{17966}{T_{s}}\right)$	Calleja et al (1981)

The total rates of each component for consumption and production can be obtained by using the following equation (Xiu et al, 2002).

$$r_{i} = \sum_{j=1}^{3} v_{ij} R_{j}$$
(17)

Where v_{ij} is the stoichiometric coefficient of the component i, in the reaction j the v_{ij} is negative for the reagent component. On the other hand, the v_{ij} is positive for the product component. Therefore, the total rate for each component was found as:

$$R_{O_2} = -R_I \tag{18}$$

$$R_{CO_2} = (R_I + R_{III}) - R_{IV}$$
⁽¹⁹⁾

$$\mathbf{R}_{\rm CO} = \left(\mathbf{R}_{\rm II} - \mathbf{R}_{\rm III}\right) + 2\mathbf{R}_{\rm IV} \tag{20}$$

$$R_{H_2} = R_{II} + R_{III}$$

$$(21)$$

$$(22)$$

$$\kappa_{\rm H_2O} = -\left(\kappa_{\rm II} + \kappa_{\rm III}\right) \tag{22}$$

The carbon molar fraction that appears in the reactions I, II and IV is calculated with relation to the combustion of the individual particles of carbon (Basu, 1999). The rate of carbon (RC) of Equation (29) was given by shrinking unreacted model (Levenspiel, 1984). The rate for this model was given by Basu and Fraser (1991) as:

$$R_{C} = \frac{PV_{O_{2}}}{T_{g}} \left(\frac{k_{m} k_{c}}{k_{c} + k_{m}} \right) Y_{O_{2}}, \ k_{m} = 12 \frac{\phi Sh D_{O_{2}}}{d_{c} R T_{m}}; \ k_{c} = 1,006 \exp\left(-\frac{7137}{T_{s}}\right)$$
(23)

4. RESULTS AND DISCUSSIONS

Equations (24)-(39) were solved with the Runge-Kutta Gill's method application (Rice and Do, 1995). In sequence, it was developed a program in the Fortran 90 language to delimit T_g , T_s , Y_{O2} , Y_{CO} , Y_{CO2} , Y_{H2O} and Y_C . The program was fed with the numerical values of the Table 2.

Table 2. Data used in the simulatio

Correlation	References
$V_{\rm mf} = \frac{V_g}{d_s \rho_g} \left\{ \left[(25,25)^2 + \frac{0,0651d_s^2 (\rho_s - \rho_g)^2 g}{\mu_g^2} \right]^{1/2} - 25,25 \right\}$	Sit e Grace, (1981)
$\varepsilon_{\rm s} = \varepsilon_{\rm mf} + 6.10 \times 10^{-4} \exp\left(\frac{V_{\rm sg} - V_{\rm mf}}{0.262}\right); \ \varepsilon_{\rm g} = 0.784 - 0.139 \exp\left(\frac{V_{\rm sg} - V_{\rm mf}}{0.272}\right)$	Cui et al., (2000)
$\varepsilon_{\rm mf} = 0.586 \left(\frac{1}{\rm Ar}\right)^{0.029} \left(\frac{\rho_{\rm g}}{\rho_{\rm s}}\right)^{0.021}$	Broadhurst e Becker (1975)
Nu _s = $(7 - 10 \epsilon_g + 5 \epsilon_g^2) (1 + 0.7 \text{ Re}_s^{0.2} \text{ Pr}_{3}^{1/3}) + \text{Re}_s^{0.7} \text{ Pr}_{3}^{1/3}$ $(1.33 - 2.4 \epsilon_g + 1.2 \epsilon_g^2)$	Syamlal et al., (1993)
$Ar = \rho_g \left(\rho_s - \rho_g \right) g \frac{d_s^3}{\mu_g^2}$	Abdullah et al., (2003)
$F_{s} = F_{s,0} x_{c}; Q_{ar} = Q_{mf,ar} (1 + \varepsilon x) \frac{T}{T_{0}} \frac{P_{0}}{P}$	Scala e Salatino (2000)
$\frac{1}{D_{i,eff}} = \frac{\varepsilon_g}{\tau} \left(\frac{1}{D_{k,i}} + \frac{1}{D_{m,i}} \right); i = O_2, \text{CO e } CO_2$	Vasconcelos et al., (2003)
$\frac{1}{h_{gs}} = \frac{1}{h_g} + \frac{1}{h_s}; \ h_g = \frac{6\lambda_{g,eff_g} Nu_s}{d_s^2}; \ h_s = \frac{2\pi^2 k_{s,eff}}{9d_s^2}$	Syamlal et al., (1993)
$Pr_{g} = \frac{C_{p,g} \mu_{g}}{\lambda_{g,eff}}; Re_{s} = \frac{d_{s} F_{s} - Q_{ar} \rho_{g}}{\mu_{g}}$	Syamlal et al., (1993)

Parameters	Values	Parameters	Values	Parameters	Values
d _s	183,356	$C_{p,g}$	$1,77 \times 10^3$	g	9,98
ρ _s	2530	$C_{P,s}$	$4,02 \times 10^3$	A _s	150
$ ho_{ m g}$	24	Р	$2,1x10^{6}$	R	8,314
$\mu_{ m g}$	1,14x10 ⁻⁵	V_{g}	0,20	Н	0,5
$\lambda_{g,eff}$	2,49x10 ⁻²	ΔH_{j}	3,835x10 ⁶	$\lambda_{s,eff}$	3,76x10 ⁻¹
T _{g,0}	500°C	$T_{s,0}$	600°C	P_{g}	$2,1x10^{6}$

Table 3. The simulation complementary parameters (Fan et al., 2003)

The T_g , T_S , Y_{O2} , Y_{CO} , Y_{CO2} , Y_{H2O} and Y_C variable behavior was shown in Figures (2), (3), (4), (5) and (6).



Figure 2. The gas phase temperature profiles for the five different drainage at the gasifier entrance



Figure 3. The solid phase temperature profiles for the five different drainage at the entrance of gasifier.



Figure 4. The components O₂, CO, CO₂, H₂ and H₂O molar fraction behavior.



Figure 5: The component C molar fraction behavior for five different drainage of the solid phase

Figures (2) and (3) showed the temperatures dynamic profiles of the gas and solid phases at exit of the fluid-solid fluidization zone. It verified a substantial increasing of temperatures T_g and T_s with the decreasing of the gas and solid drainages at the entrance of gasifier. The Figure 2 shown that the gas temperature reaches the stationary state in $t = \pm$ 60s for a gas drainage, $Q_{g,0} = 20 \times 10^{-4} \text{ m}^3 \text{ s}^{-1}$, reaching a temperature of $\pm 1200^{\circ}\text{C}$. The Figure (4) shows the behavior of the reagent and product components of the gasification process. In Figure (5), it was analyzed the behavior of the carbon component behavior for five solid drainage. On the other hand, the Figure (6) showed a validation case.



Figure 6: Numerical cases validation with the literature result

5. CONCLUSIONS

The forecasts of the temperatures behavior of the gaseous phase and of the solid phase, as well as of the components O_2 , CO, CO_2 , H_2O , H_2O , H_2 and C were shown in this work. For such end, it developed a mathematical model for variable Tg, Ts, Y_{O2} , Y_{CO2} , Y_{H2O} , Y_{H2O} , Y_{H2} and Y_C . The mathematical model simulation supplied the behavior of these you varied, driving the following conclusions:

- The developed model allowed to analyze the variable Tg sensibility with different drainage of entrance of the gas (Qar,0), as well as it allowed to verify the variable Ts sensibility with different drainage of entrance Fs,0.
- The sewage Qar,0 and Fs,0 of entrance presented strong influence on variable Tg, Ts, YO2, YCO, YCO2 and YC, should be consumed in the control of LF.

6. NOMENCLATURE

- A_s Gasifier cross area, m²
- $C_{p, g}$ Gas heat capacity, J/K mol
- $C_{p,s}$ Solid heat capacity, J/K mol
- D_i ,eff Effective diffusion coefficient, m²/s
- F_s Mass flux of solid, kg/s
- h_{gs} Gas-solid transfer coefficient of solid, W/m² K
- ΔH_r Entalpy of reaction, kJ/mol
- Q_g Total volumeter flow rate, m³/s
- $\vec{R_i}$ Reaction rates for the component, $i = O_2$, CO, CO₂, H₂O and H₂, $\vec{s^{-1}}$
- t time, s^{-1}
- T_g Gas temperature, K
- T_s Solid temperature, K
- Y_c Carbon molar fraction, dimensionless
- Y_i Molar fraction for the component $i = O_2$, CO, CO₂, H₂O and H₂, dimensionless

6.1. Greek Letters

- ϵ_g The gas fraction volume, dimensionless
- ϵ_{s} Bed porosity, dimensionless
- $\rho_{\rm g}$ Gas density, kg/m³
- ρ_s solid density, kg/m³
- $\lambda_{g,eff}$ The gas effective heat conductivity, J/m s K
- $\lambda_{s,ef}$ The solid effective heat conductivity, J/m s K

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APPENDIX-A

Table A1: Entrance and Parameter variables α_1 , α_2 , β_1 , β_2 , β_3 e β_4

$\left. T_{g} \right _{z = 0^{-}} (t) = T_{ent, g}$	$\left. T_{s} \right _{z = 0} - (t) = T_{ent,s}$
$Y_{O_2, ar}(t) \Big _{z = 0^{-}} = Y_{O_2, ar}^{0}$	$Y_{CO, ar}(t)\Big _{z=0} = Y_{CO, ar}^{0}$
$Y_{CO_{2}ar}(t)\Big _{z=0} = Y_{CO_{2}ar}^{0}$	$Y_{C,ar}(t)\Big _{z=0^{-}} = Y_{C,ar}^{0}$
$\alpha_1 = \frac{\rho_g C_{p,g} Q_{ar} \Delta z}{\lambda_{g,eff} A_s}$	$\alpha_2 = \frac{\rho_s C_{p,s} F_s \Delta z}{\lambda_{s,eff} A_s}$
$\beta_1 = \frac{Q_{ar}}{A_s} \frac{\Delta z}{D_{O_2, eff}}$	$\beta_2 = \frac{Q_{ar}}{A_s} \frac{\Delta z}{D_{CO,eff}}$
$\beta_3 = \frac{Q_{ar}}{A_s} \frac{\Delta z}{D_{CO_2, eff}}$	$\beta_4 = \frac{Q_{ar}}{A_s} \frac{\Delta z}{D_{C, eff}}$