MATHEMATICAL MODELING, COMPUTER SIMULATION AND OPTIMIZATION OF A GASIFICATION UNIT FOR FUEL GAS GENERATION

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Abstract.*The energy recycling process is essential for energy development and improvement of environmental infrastructure of any country. This recycling process can be made by the fluidized bed gasifier, major equipment for the gasification process. This equipment involves both solid and gaseous phases. The solid phase can be inserted laterally into the bed and the gaseous phase may be introduced through the bottom of the gasifier by means of a blower and uniformly distributed along the bed through a distributor plate. In this context, this research aims to analyze the behavior of steady state chemical components in the reduction zone of a fluidized bed gasifier using a mathematical model simulation. These components are carbon monoxide (CO), carbon dioxide (CO_2), water vapor (H_2O), hydrogen (H_2), methane (CH_4) and carbon ($C_{(s)}$). The gasification process, however, is very complex and thecomponents analysis in the region of reduction involves balance equations for the species CO, CO_2, H_2O, H_2, CH_4 and $C_{(s)}$ forming a system of ordinary differential equations (ODE) coupled. This system can be solved by several known methods that aim to discretize the derivatives and for this we will usethe finite difference method.*

Keywords: gasifier, mathematical modeling, fuel generation, simulation.

1. INTRODUCTION

The global concern with the depletion of fossil fuels and rising environmental problems associated with the use of these sources has attracted the attention of researchers to develop new processes for power generation based on renewable sources. Biomass has been considered a renewable energy source. Alternatively, the biomass can be converted into gaseous fuel through gasification technology (Oliveira and Silva, 2013).

In the biomass gasification process the fluidized bed gasifier is the main equipment responsible for the fuel gas production through cane sugar bagasse. Gasification is defined as the biomass or any solid fuel conversion into an energy gas by partial oxidation at elevated temperatures. This conversion can be made in several types of reactors, such as fixed bed and fluidized bed reactors (Gumz, 1950). The produced gas in our case a CO and H_2 mixture has many practical applications, such as combustion in engines or turbines for power generation, electric power, irrigation pumps for the direct generation of heat and raw material in the chemical synthesis of ammonia and methane.

A fluidized bed is a mass of fine grained material which is kept in suspension by an upward gas stream. The fluid beds are used in the chemical industry and utilized to promote rapid heating and mixing fluids, resulting in well-controlled reactions and usually quick. The bed material may be a reagent, a catalyst or an inert material such as sand (Neiva, 1987). The fuel particles are kept suspended in a bed of inert particles (sand, ash, alumina, etc.) and fluidized by air flow. The biomass is fed into small dimensions to the fluidization happen (Hector and Whitelaw, 1986) (Kreinin and Shifrin, 1993). The gasification process is very complex. However, components analysis at the reduction zone involves balance equations for the species CO, CO_2, H_2O, H_2, CH_4 and $C_{(s)}$ forming a system of ordinary differential equations (ODEs) coupled. This system can be solved by various methods known in the literature, which aims to discretize the derivatives (Silva and Lucena, 2007).

In this paper we will start with the mathematical modeling using the finite difference method. Once we have the discretized equations we can solve them and make computational simulation. At last we will bring the sensitivity analysis and make some conclusions about the gasifier's parameters that can influence most significantly in the fuel gas production.

2. MATHEMATICAL MODELING

In order to describe in a simplified way the processes happening in the reduction zone of the gasiefer, we consider only three following heterogeneous chemical equations:

$$C + CO_2 \Leftrightarrow 2\,CO \tag{1}$$

$$C + H_2O \Leftrightarrow CO + H_2 \tag{2}$$

$$C + 2H_2 \Leftrightarrow CH_4 \tag{3}$$

The whole mathematical modeling developed was based on the mass transfer in the reduction zone of a fluidized bed gasifier, with greater emphasis on analyzing the components CO and H2. Therefore, whenever we refer to the gasifier, is subtended that we are talking about the reduction zone of fluidized bed gasifier.

To simplify the mass balance equations we propose the following hypothesis: stationary system; one-dimensional model for the mass balance; isothermal gasification system; mass balance of the components modeled by observing the effect of axial dispersion. The ordinary differential equations and the boundary conditions of each component below are the mass balance equations that characterize the system behavior.

Mass balance for CO:

$$D_{CO,eff}\frac{d^2\left(\varepsilon_g\,\rho_g\,Y_{CO}\right)}{dz^2} - \frac{Q_g}{A_s}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{CO}\right)}{dz} + \frac{R\,T_g}{P}\,R_{CO} = 0 \tag{4}$$

Boundary conditions for CO:

$$D_{CO,eff}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{CO}\right)}{dz}\bigg|_{z=0^+} = \frac{Q_g}{A_S}\left[\left(\varepsilon_g\,\rho_g\,Y_{CO}\right)\big|_{z=0^+} - \left(\varepsilon_g\,\rho_g\,Y_{CO,0}\right)\right] \tag{5}$$

$$D_{CO,eff}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{CO}\right)}{dz}\bigg|_{z=L} = 0 \tag{6}$$

Mass balance for CO_2:

$$D_{CO_2,eff}\frac{d^2\left(\varepsilon_g\,\rho_g\,Y_{CO_2}\right)}{dz^2} - \frac{Q_g}{A_s}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{CO_2}\right)}{dz} + \frac{R\,T_g}{P}\,R_{CO_2} = 0 \tag{7}$$

Boundary conditions for CO_2:

$$D_{CO_2,eff}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{CO_2}\right)}{dz}\bigg|_{z=0^+} = \frac{Q_g}{A_S}\left[\left(\varepsilon_g\,\rho_g\,Y_{CO_2}\right)\big|_{z=0^+} - \left(\varepsilon_g\,\rho_g\,Y_{CO_2,0}\right)\right] \tag{8}$$

$$D_{CO,eff}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{CO_2}\right)}{dz}\bigg|_{z=L} = 0 \tag{9}$$

Mass balance for H_2O:

$$D_{H_2O,eff}\frac{d^2\left(\varepsilon_g\,\rho_g\,Y_{H_2O}\right)}{dz^2} - \frac{Q_g}{A_s}\frac{d\left(\varepsilon_g\,\rho_g\,Y_{H_2O}\right)}{dz} + \frac{R\,T_g}{P}\,R_{H_2O} = 0 \tag{10}$$

Boundary conditions for H_2O:

$$D_{H2O,eff} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{H_2O}\right)}{dz}\bigg|_{z=0^+} = \frac{Q_g}{A_S}\left[\left(\varepsilon_g \rho_g Y_{H_2O}\right)\big|_{z=0^+} - \left(\varepsilon_g \, \rho_g \, Y_{H_2O,0}\right)\right] \tag{11}$$

$$D_{CO,eff} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{H_2O}\right)}{dz}\bigg|_{z=L} = 0 \tag{12}$$

Mass balance for H_2:

$$D_{H2,eff} \frac{d^2\left(\varepsilon_g \, \rho_g \, Y_{H_2}\right)}{dz^2} - \frac{Q_g}{A_s} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{H_2}\right)}{dz} + \frac{R \, T_g}{P} R_{H_2} = 0 \tag{13}$$

Boundary conditions for H_2:

$$D_{H2,eff} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{H_2}\right)}{dz}\bigg|_{z=0^+} = \frac{Q_g}{A_S}\left[\left(\varepsilon_g \rho_g Y_{H_2}\right)\big|_{z=0^+} - \left(\varepsilon_g \, \rho_g \, Y_{H2,0}\right)\right] \tag{14}$$

$$D_{H2,eff} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{H_2}\right)}{dz}\bigg|_{z=L} = 0 \tag{15}$$

Mass balance for CH_4:

$$D_{CH4,eff} \frac{d^2\left(\varepsilon_g \, \rho_g \, Y_{CH4}\right)}{dz^2} - \frac{Q_g}{A_s} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{CH4}\right)}{dz} + \frac{R \, T_g}{P} R_{CH4} = 0 \tag{16}$$

Boundary conditions for CH_4:

$$D_{CH4,eff} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{CH4}\right)}{dz}\bigg|_{z=0^+} = \frac{Q_g}{A_S}\left[\left(\varepsilon_g \rho_g Y_{CH4}\right)\big|_{z=0^+} - \left(\varepsilon_g \, \rho_g \, Y_{CH4,0}\right)\right] \tag{17}$$

$$D_{CH4,eff} \frac{d\left(\varepsilon_g \, \rho_g \, Y_{CH_2}\right)}{dz}\bigg|_{z=L} = 0 \tag{18}$$

Mass balance for C:

$$D_{C,eff} \frac{d^2\left(\varepsilon_s \, \rho_s Y_C\right)}{dz^2} - \frac{G_s}{A_s} \frac{d\left(\varepsilon_s \, \rho_s Y_C\right)}{dz} - 3\frac{R \, T_g}{P} R_C = 0 \tag{19}$$

Boundary conditions for C:

$$D_{C,eff} \frac{d\left(\varepsilon_s \, \rho_s Y_C\right)}{dz}\bigg|_{z=0^+} = \frac{G_s}{A_S}\left[\left(\varepsilon_s \rho_s Y_C\right)\big|_{z=0^+} - \left(\varepsilon_s \, \rho_s Y_{C,0}\right)\right] \tag{20}$$

$$D_{C,eff} \frac{d\left(\varepsilon_s \, \rho_s Y_C\right)}{dz}\bigg|_{z=L} = 0 \tag{21}$$

The physical quantities in the equations above are:

$D_{i,eff}$: Diffusion coefficient of i component, $i = CO, CO_2, H_2O, H_2, CH_4, C_{(s)}$, m^{2}s^{-1};
Y_i: Mole fractions of i component, $i = CO, CO_2, H_2O, H_2, CH_4, C_{(s)}$;
ε_g: Gaseous void fraction;
ε_s: Solid void fraction;
ρ_g: Gas density, kg m^{-3};
ρ_s: Particle density, kg m^{-3};
Q_g: Gas flow rate, m^{3}s^{-1};
G_s: Coal feed rate, m^{3}s^{-1};
A_s: Gas-solid specific area per unit volume of the gasification region, m^{-1};
R: Gas Constant, J mol^{-1}K^{-1};
P: Pressure, Pa;
T_g: Gas temperature, K.

Continuing with the mathematical discretization methodology used in this research, we obtain the discretized equations below, with alpha (α) and beta (β) parameters detailed in Tab. 1:

$$\beta_{1,CO}(Y_{CO})_j - \beta_{1,CO}(Y_{CO,0}) + \alpha_{3,CO}(R_{CO})_j = 0 \tag{22}$$

$$\beta_{1,CO_2}(Y_{CO_2})_j - \beta_{1,CO_2}(Y_{CO_2,0}) + \alpha_{3,CO_2}(R_{CO_2})_j = 0 \tag{23}$$

$$\beta_{1,H_2O}(Y_{H_2O})_j - \beta_{1,H_2O}(Y_{H_2O,0}) + \alpha_{3,H_2O}(R_{H_2O})_j = 0 \tag{24}$$

$$\beta_{1,H_2}(Y_{H_2})_j - \beta_{1,H_2}(Y_{H_2,0}) + \alpha_{3,H_2}(R_{H_2})_j = 0 \tag{25}$$

$$\beta_{1,CH_4}(Y_{CH_4})_j - \beta_{1,CH_4}(Y_{CH_4,0}) + \alpha_{3,CH_4}(R_{CH_4})_j = 0 \tag{26}$$

$$\beta_{1,C}(Y_C)_j - \beta_{1,C}(Y_{C,0}) + \alpha_{3,C}(R_C)_j = 0 \tag{27}$$

Table 1. Alpha (α) and beta (β) parameters.

Components	Parameters (α)	Parameters (β)
CO	$\alpha_{1,CO} = D_{CO,eff}\,\varepsilon_g\,\rho_g$; $\alpha_{2,CO} = \dfrac{Q_g\varepsilon_g\,\rho_g}{A_s}$; $\alpha_{3,CO} = \dfrac{R\,T_g}{P}$	$\beta_{1,CO} = \dfrac{2(\alpha_{2,CO})^3\,\Delta z}{(\alpha_{2,CO}\Delta z)^2 - 4(\alpha_{1,CO})^2}$
CO$_2$	$\alpha_{1,CO_2} = D_{CO_2,eff}\,\varepsilon_g\,\rho_g$; $\alpha_{2,CO_2} = \dfrac{Q_g\varepsilon_g\,\rho_g}{A_s}$; $\alpha_{3,CO_2} = \dfrac{R\,T_g}{P}$	$\beta_{1,CO_2} = \dfrac{2(\alpha_{2,CO_2})^3\,\Delta z}{(\alpha_{2,CO_2}\Delta z)^2 - 4(\alpha_{1,CO_2})^2}$
H$_2$O	$\alpha_{1,H_2O} = D_{H_2O,eff}\,\varepsilon_g\,\rho_g$; $\alpha_{2,H_2O} = \dfrac{Q_g\varepsilon_g\,\rho_g}{A_s}$; $\alpha_{3,H_2O} = \dfrac{R\,T_g}{P}$	$\beta_{1,H_2O} = \dfrac{2(\alpha_{2,H_2O})^3\,\Delta z}{(\alpha_{2,H_2O}\Delta z)^2 - 4(\alpha_{1,H_2O})^2}$
H$_2$	$\alpha_{1,H_2} = D_{H_2,eff}\,\varepsilon_g\,\rho_g$; $\alpha_{2,H_2} = \dfrac{Q_g\varepsilon_g\,\rho_g}{A_s}$; $\alpha_{3,H_2} = \dfrac{R\,T_g}{P}$	$\beta_{1,H_2} = \dfrac{2(\alpha_{2,H_2})^3\,\Delta z}{(\alpha_{2,H_2}\Delta z)^2 - 4(\alpha_{1,H_2})^2}$
CH$_4$	$\alpha_{1,CH_4} = D_{CH_4,eff}\,\varepsilon_g\,\rho_g$; $\alpha_{2,CH_4} = \dfrac{Q_g\varepsilon_g\,\rho_g}{A_s}$; $\alpha_{3,CH_4} = \dfrac{R\,T_g}{P}$	$\beta_{1,CH_4} = \dfrac{2(\alpha_{2,CH_4})^3\,\Delta z}{(\alpha_{2,CH_4}\Delta z)^2 - 4(\alpha_{1,CH_4})^2}$
C	$\alpha_{1,C} = D_{C,eff}\,\varepsilon_s\,\rho_s$; $\alpha_{2,C} = \dfrac{G_s\varepsilon_s\,\rho_s}{A_s}$; $\alpha_{3,C} = -3\dfrac{R\,T_g}{P}$	$\beta_{1,C} = \dfrac{2(\alpha_{2,C})^3\,\Delta z}{(\alpha_{2,C}\Delta z)^2 - 4(\alpha_{1,C})^2}$

2.1. Mathematical Model Development

The rates of the reactions of gaseous components formation, Eq. (01), (02) and (03), are shown below:

$$R_I = k_1 \left(\frac{P}{R\,T_g} \right) Y_{CO_2} \tag{28}$$

$$R_{II} = 2\,k_2 \left(\frac{P}{R\,T_g} \right) Y_{H_2O} \tag{29}$$

$$R_{III} = 0{,}1\,k_3 \left(\frac{P}{R\,T_g} \right) Y_{H_2} \tag{30}$$

The total rate of formation and consumption for each component was obtained using the following equation (Xiu et al. 2002):

$$r_i = \sum_{j=1}^{3} v_{ij}\,R_j \tag{31}$$

where v_{ij} is the stoichiometric coefficient of i component in j reaction. If v_{ij} is a reagent, v_{ij} assumes a negative sign, but if v_{ij} is a product, a positive sign. Using this technique, the overall rates of reaction for each component are:

$$R_{CO} = 2\,R_I + R_{II} \tag{32}$$

$$R_{CO_2} = -R_I \tag{33}$$

$$R_{H_2O} = -R_{II} \tag{34}$$

$$R_{H_2} = R_{II} - 2\,R_{III} \tag{35}$$

$$R_{CH_4} = R_{III} \tag{36}$$

$$R_C = -R_I - R_{II} - R_{III} \tag{37}$$

By substituting the rates for reactions (I, II and III) in the reactions for each component we obtain rates of the components as a function of the constants k_1, k_2 and k_3 and concentrations of each component, resulting in the following equations:

$$R_{CO} = 2\,k_1 \left(\frac{P}{R\,T_g} \right) Y_{CO_2} + 2\,k_2 \left(\frac{P}{R\,T_g} \right) Y_{H_2O} \tag{38}$$

$$R_{CO_2} = -k_1 \left(\frac{P}{R\,T_g} \right) Y_{CO_2} \tag{39}$$

ISSN 2176-5480

Daniel Lucena de Athayde Guimarães and Jornandes Dias da Silva
Mathematical Modeling, Computer Simulation and Optimization of a Gasification Unit for Fuel Gas Generation

$$R_{H_2O} = -2k_2\left(\frac{P}{R\,T_g}\right)Y_{H_2O} \tag{40}$$

$$R_{H_2} = 2k_2\left(\frac{P}{R\,T_g}\right)Y_{H_2O} - 0{,}2\,k_3\left(\frac{P}{R\,T_g}\right)Y_{H_2} \tag{41}$$

$$R_{CH_4} = 0{,}1\,k_3\left(\frac{P}{R\,T_g}\right)Y_{H_2} \tag{42}$$

$$R_C = -k_1\left(\frac{P}{R\,T_g}\right)Y_{CO_2} - 2k_2\left(\frac{P}{R\,T_g}\right)Y_{H_2O} - 0{,}1\,k_3\left(\frac{P}{R\,T_g}\right)Y_{H_2} \tag{43}$$

Following this the next step of the modeling is to replace the Eq. (38) to (43) in Eq. (22) to (27). Once we have done this we obtain the following equations:

$$\beta_{1,CO}(Y_{CO})_j + 2k_1\left(Y_{CO_2}\right)_j + 2k_2\left(Y_{H_2O}\right)_j = \beta_{1,CO}(Y_{CO,0}) \tag{44}$$

$$\left(\beta_{1,CO_2} - k_1\right)\!\left(Y_{CO_2}\right)_j = \beta_{1,CO_2}\left(Y_{CO_2,0}\right) \tag{45}$$

$$\left(\beta_{1,H_2O} - 2k_2\right)\!\left(Y_{H_2O}\right)_j = \beta_{1,H_2O}\left(Y_{H_2O,0}\right) \tag{46}$$

$$2k_2\left(Y_{H_2O}\right)_j + \left(\beta_{1,H_2} - 0{,}2\,k_3\right)\!\left(Y_{H_2}\right)_j = \beta_{1,H_2}\left(Y_{H_2,0}\right) \tag{47}$$

$$0{,}1\,k_3\left(Y_{H_2}\right)_j + \beta_{1,CH_4}\left(Y_{CH_4}\right)_j = \beta_{1,CH_4}\left(Y_{CH_4,0}\right) \tag{48}$$

$$3k_1\left(Y_{CO_2}\right)_j + 6k_2\left(Y_{H_2O}\right)_j + 0{,}3\,k_3\left(Y_{H_2}\right)_j + \beta_{1,C}(Y_C)_j = \beta_{1,C}(Y_{C,0}) \tag{49}$$

2.2. Numerical Methodology

The model equations and reaction rates are a system of nonlinear second order differential equations featuring a boundary value problem. Just for remember, for the linearization and discretization of the equations we used the finite difference method and because of the complexity of solving these equations by analytical means was employed the over-relaxation numerical method.

To obtain the gases generated behavior inside the gasifier we applied the over-relaxation method. The following are the equations of the reduction zone in the fluidized bed gasifier for the effect of mass transfer, expressed as a function of the parameters a and b.

$$a_{11}(Y_{CO})_j + a_{12}\left(Y_{CO_2}\right)_j + a_{13}\left(Y_{H_2O}\right)_j + a_{14}\left(Y_{H_2}\right)_j + a_{15}\left(Y_{CH_4}\right)_j + a_{16}(Y_C)_j = b_1 \tag{50}$$

$$a_{21}(Y_{CO})_j + a_{22}\left(Y_{CO_2}\right)_j + a_{23}\left(Y_{H_2O}\right)_j + a_{24}\left(Y_{H_2}\right)_j + a_{25}\left(Y_{CH_4}\right)_j + a_{26}(Y_C)_j = b_2 \tag{51}$$

$$a_{31}(Y_{CO})_j + a_{32}\left(Y_{CO_2}\right)_j + a_{33}\left(Y_{H_2O}\right)_j + a_{34}\left(Y_{H_2}\right)_j + a_{35}\left(Y_{CH_4}\right)_j + a_{36}(Y_C)_j = b_3 \tag{52}$$

$$a_{41}(Y_{CO})_j + a_{42}\left(Y_{CO_2}\right)_j + a_{43}\left(Y_{H_2O}\right)_j + a_{44}\left(Y_{H_2}\right)_j + a_{45}\left(Y_{CH_4}\right)_j + a_{46}(Y_C)_j = b_4 \tag{53}$$

$$a_{51}(Y_{CO})_j + a_{52}(Y_{CO_2})_j + a_{53}(Y_{H_2O})_j + a_{54}(Y_{H_2})_j + a_{55}(Y_{CH_4})_j + a_{56}(Y_C)_j = b_5 \tag{54}$$

$$a_{61}(Y_{CO})_j + a_{62}(Y_{CO_2})_j + a_{63}(Y_{H_2O})_j + a_{64}(Y_{H_2})_j + a_{65}(Y_{CH_4})_j + a_{66}(Y_C)_j = b_6 \tag{55}$$

Table 2. a Parameters of Eq. (50) to (55).

$a_{11} = \beta_{1,CO}$	$a_{62} = 2k_1$	$a_{13} = 2k_2$	$a_{14} = 0$	$a_{15} = 0$	$a_{16} = 0$
$a_{21} = 0$	$a_{22} = \beta_{1,CO_2} - k_1$	$a_{23} = 0$	$a_{24} = 0$	$a_{25} = 0$	$a_{26} = 0$
$a_{31} = 0$	$a_{32} = 0$	$a_{33} = \beta_{1,H_2O} - 2k_2$	$a_{34} = 0$	$a_{35} = 0$	$a_{36} = 0$
$a_{41} = 0$	$a_{42} = 0$	$a_{43} = 2k_2$	$a_{44} = \beta_{1,H_2} - 0,2k_3$	$a_{45} = 0$	$a_{46} = 0$
$a_{51} = 0$	$a_{52} = 0$	$a_{53} = 0$	$a_{54} = 0.1k_3$	$a_{55} = \beta_{1,CH_4}$	$a_{56} = 0$
$a_{61} = 0$	$a_{62} = 3k_1$	$a_{63} = 6k_2$	$a_{64} = 0.3k_3$	$a_{65} = 0$	$a_{66} = \beta_{1,C}$

Table 3. b Parameters of Eq. (50) to (55).

$b_1 = \beta_{1,CO}Y_{CO,0}$	$b_2 = \beta_{1,CO_2}Y_{CO2,0}$	$b_3 = \beta_{1,H_2O}Y_{H_2O,0}$
$b_4 = \beta_{1,H_2}Y_{H2,0}$	$b_5 = \beta_{1,CH_4}Y_{CH4,0}$	$b_6 = \beta_{1,C}Y_{C,0}$

3. RESULTS AND DISCUSSIONS

Applying the over-relaxation numerical method we obtained the behavior of gases generated and consumed in terms of mole fractions throughout the reduction zone of the gasifier. All parameters used in the computer simulation are shown in Tab. 4 and the results presented in the Fig. 1 and 2 following.

Table 4. Input values of operating conditions, properties of the gas and solid phases used in the simulation (Oliveira and Silva, 2013)

| Categories	Properties	Numerical Values
Operation Conditions	Operation temperature of the gas phase, Tg K	750
	Operation temperature of the solid phase, Ts K	750
	Operation pressure, P Pa	1.013×10^5
	Gas flow rate, Q_g m³ s⁻¹	9.500×10^{-1}
	Coal feed rate, G_s m³s⁻¹	3.060×10^{-2}
	Gas-solid specific area per unit volume of the gasification region, A_s m⁻¹	125
	Initial mole fraction of CO, $Y_{CO,0}$ (-)	0.000
	Initial mole fraction of CO_2, $Y_{CO2,0}$ (-)	0.300
	Initial mole fraction of H_2O, $Y_{H2O,0}$ (-)	0.200
	Initial mole fraction of H_2, $Y_{H2,0}$ (-)	0.000
	Initial mole fraction of CH_4, $Y_{CH4,0}$ (-)	0.150
	Initial mole fraction of $C_{(s)}$, $Y_{C,0}$ (-)	0.250
Gas properties	Void fraction of the gaseous phase, ε_g (-)	0.430
	Density of the gaseous phase, ρ_g kg m⁻³	0.500
	Diffusion coefficient of CO, $D_{CO,eff}$ m² s⁻¹	2.500×10^{-5}
	Diffusion coefficient for CO_2, $D_{CO2,eff}$ m² s⁻¹	1.400×10^{-5}
	Diffusion coefficient of H_2O, $D_{H2O,eff}$ m² s⁻¹	2.800×10^{-5}
	Diffusion coefficient of H_2, $D_{H2,eff}$ m² s⁻¹	4.103×10^{-5}
	Diffusion coefficient of CH_4, $D_{CH4,eff}$ m² s⁻¹	5.020×10^{-5}
	Diffusion coefficient for $C_{(s)}$, $D_{C(s),eff}$ m² s⁻¹	1.150×10^{-5}
Properties of the solid phase	Void fraction of the solid phase, ε_s (-)	0.630
	Density of the solid phase, ρ_s kg m⁻³	2.500×10^3
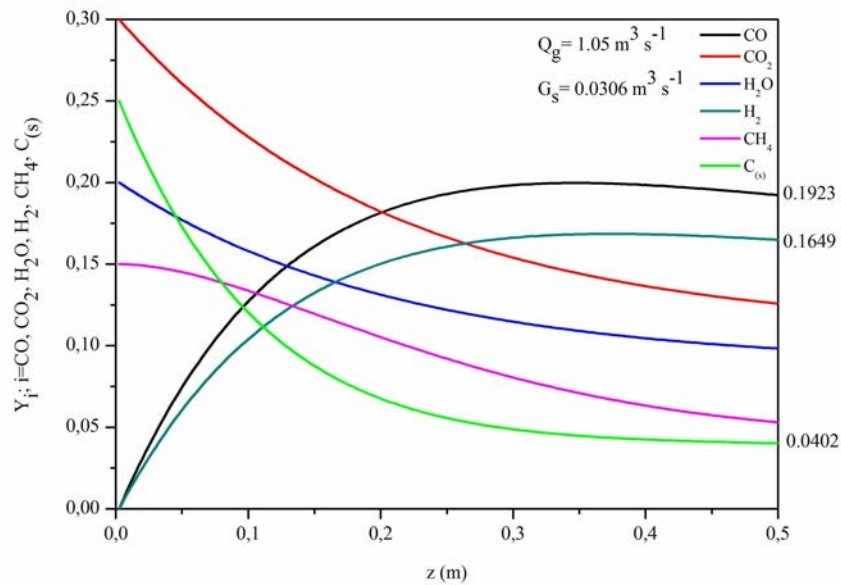
Figure 1. Profiles of the mole fractions of chemical species CO, CO_2, H_2O, H_2, CH_4, $C_{(s)}$ as a function of the distance of the gasifier beginning.
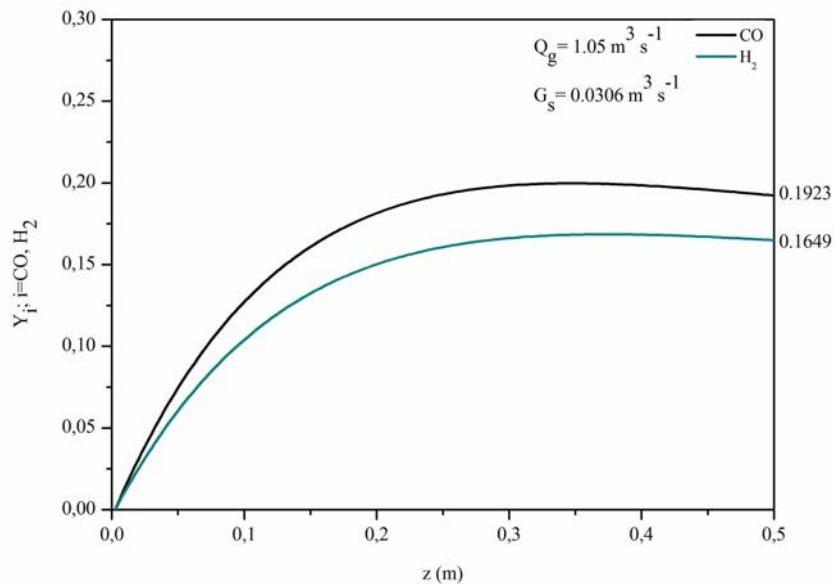

Figure 2. Profiles of the fuel gas production, CO and H_2, as a function of the distance of the gasifier beginning. The CO production stops at 0.1923 and the H_2 production stops at 0.1649.

3.1. Sensitivity Analysis

During the simulation we could see that the profiles of the components are mainly affected by gas flow rate (Q_g) and coal feed rate (G_s). Less significantly, the void fractions and density of the gas and the solid (ε_g, ε_s, ρ_g, ρ_s) can also modify the results. The results and comments are shown in the Fig. 3 to 6 following.
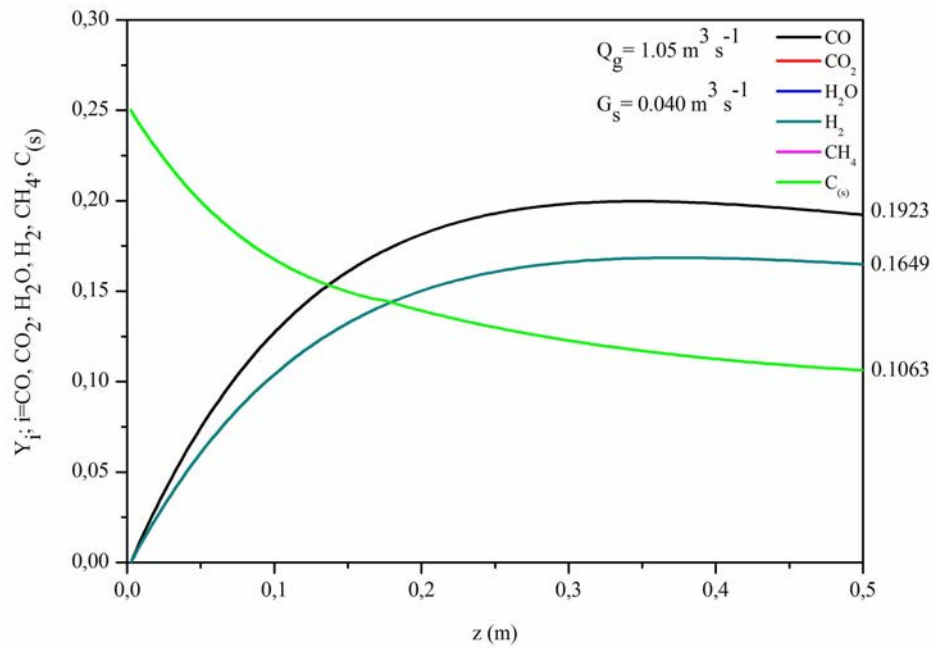
Figure 3. Profiles of the mole fractions of the fuel gas CO and H_2, and mole fraction of biomass $C_{(s)}$, as a function of the distance of the gasifier beginning. Increasing the coal feed rate we can see the carbon remaining.
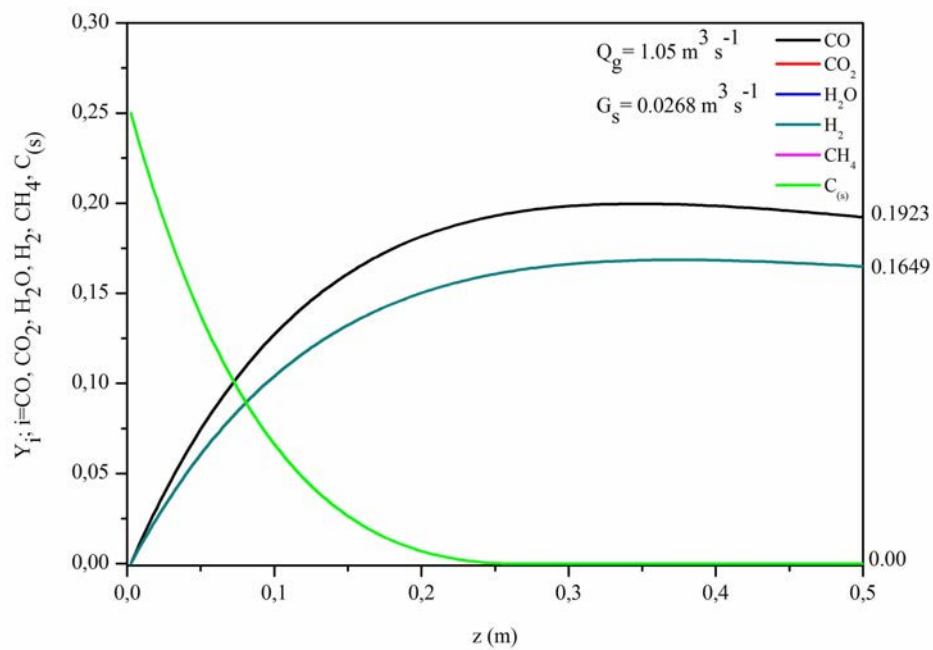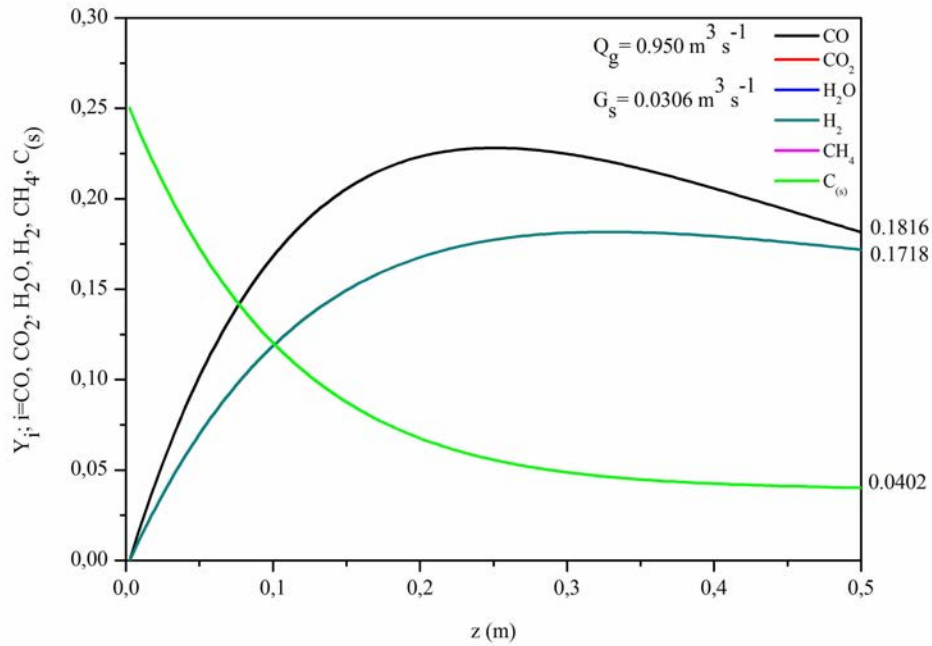

Figure 4. Profiles of the mole fractions of the fuel gas CO and H_2, and mole fraction of biomass $C_{(s)}$, as a function of the distance of the gasifier beginning. Decreasing the coal feed rate we can see that there is no carbon remaining.

Daniel Lucena de Athayde Guimarães and Jornandes Dias da Silva
Mathematical Modeling, Computer Simulation and Optimization of a Gasification Unit for Fuel Gas Generation

Figure 5. Profiles of the mole fractions of the fuel gas CO and H_2, and mole fraction of biomass $C_{(s)}$, as a function of the distance of the gasifier beginning. Decreasing the gas flow rate we can see the increase of H_2 production and the decrease of the CO production.
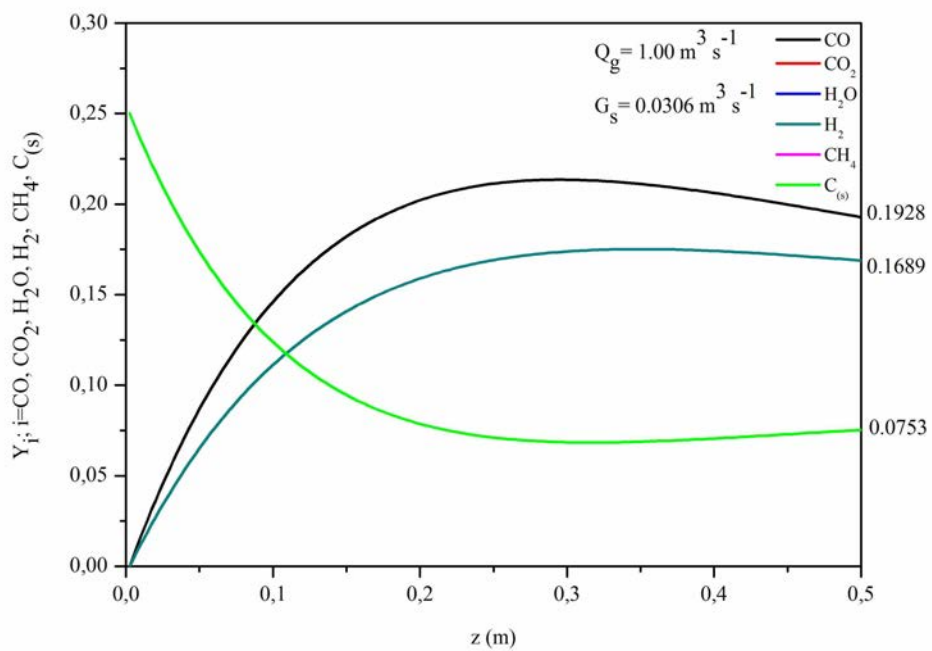

Figure 6. Profiles of the mole fractions of the fuel gas CO and H_2, and mole fraction of biomass $C_{(s)}$, as a function of the distance of the gasifier beginning. With a middle value for the gas flow rate, in relation to with Fig. 3 and 5, we can see a little increase in both CO and H_2 production.

4. CONCLUSIONS

Once we have made the sensitivity analysis The Following Conclusions can be made:

• The CO production stops near to 0.19 and on the other hand the H_2 productions stops between 0.16 and 0.17.
• By lowering the gas flow rate (Q_g) there is a decrease in the CO production and an increased in H2 production, so the gas flow rate (Q_g) can be adjusted considering which gas is wished to produce.
• The CO production is directly proportional to the gas flow rate (Q_g) and the H_2 production is inversely proportional.
• The way the carbon is consumed greatly varies with respect to the coal feed rate (G_s). In general, for the same gas flow rate (Q_g), smaller values of coal feed rate (G_s) make the $C_{(s)}$ be consumed completely.
• We could not achieve the optimum production, but the result which comes closest is shown in Fig. 1.
• The research is promising and new related studies can be developed using it as a base.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE

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