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A general mathematical model for a moving bed gasifier

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Abstract

Cocurrent and countercurrent units are common configuration of biomass and coal gasifiers. Moving solid beds contact a flowing gas phase, usually air, steam or their mixtures. Batch and fluidized bed reactors, or drop tube gasifiers are also alternative units. The complexity of these systems relies in several aspects: the chemistry of the released species in the first devolatilization and gasification step, the large number of species and reactions in the gas phase, the definition of a well balanced description of the gasifier and finally the necessity to adopt a stable ODE solver to numerically handle the large system of balance equations. The different process units are schematized in terms of a series of elementary cells where the solid particles release volatile components with effective material and energy exchanges with the flowing gas phase. Gasification reactions in the coal or biomass particles are properly accounted including mass and thermal diffusion limitations. Reactions in the gas phase are finally accounted by using a detailed kinetic scheme of pyrolysis and combustion reactions. Preliminary comparisons with experimental measurements support the proposed approach.

Keywords: Gasification, Combustion, Mathematical modeling, Biomass.

1. Introduction

Although pioneer works on gasifier modeling date the seventies (Anthony and Howard 1976) only recently a higher publication frequency appeared in literature. This is probably due to a continuous demand of alternative and renewable fuels as a consequence of a lower availability of canonical raw materials. The approaches adopted for modeling such equipment, largely vary with the applications: from thermochemical equilibrium models (Ruggiero and Manfrida 1999, Jayah et al. 2003) to very detailed CFD descriptions (Gao et al. 2006, Watanabe and Otaka 2006). Independently on the approach chosen, it seems that a low attention has been paid to mass and thermal diffusion limitations, which limit the release of volatile components and the successive reactions on the gas phase. In addition to this fact a necessary compromise between details and assumptions in model description has not been yet clearly stated. Aim of this paper is to contribute to the solution of these existing problems and a mechanistic and intrinsic model at the particle scale is presented. Although a moving bed is the most common configuration of a gasifier it is worth to include it in a framework of ancillary configurations that may be encountered as valid process alternatives.

2. Kinetic Models

It is necessary to distinguish two different kinetic models: the devotalilization, gasification and combustion in the solid particle and the pyrolysis and combustion in the gas phase. The biomass devolatilization, gasification and combustion scheme refers to about 30 species and 25 global reactions (Cuoci et al., 2007). The gas phase kinetic

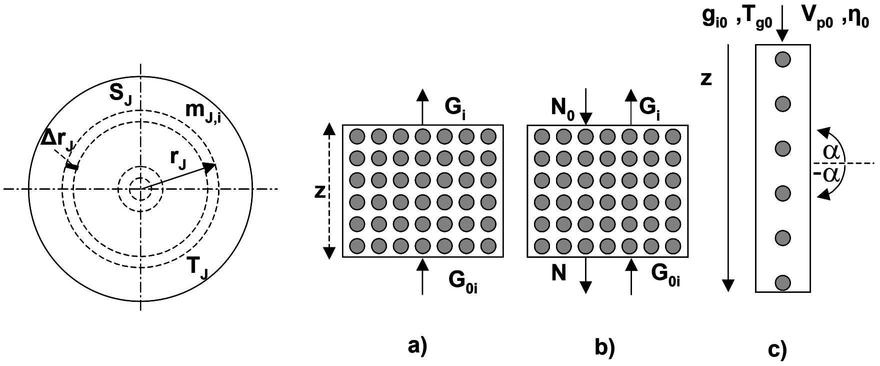

Fig.1 Particle and Gasifier sketches, a) Fixed bed, b) Moving bed, c) Drop tube

model has been extensively validated by Ranzi et al. (2001) and refers to more than 100 species involved in thousands of elementary and lumped reactions. Due to limited space available, the kinetic model will be only referenced and is available as supplementary material.

3. Reactor and particle model

Fig. 1 sketches the solid particle and three configurations of different reactors.

The particle is supposed of spherical shape, divided into NR spherical sectors (j =1 to NR). The components are supposed to be NCP, identified by *i* =1 to NCP. ‘ Sector *j*’ means the particle volume included within the radius r_j and r_{j-1}.

3.1. Fixed bed (or semi-Batch Reactor)

Fig. 1. a) sketches the reactor bed that is supposed divided along its vertical axis into a defined number of elements. Here for sake of simplicity in exposition a single element is assumed. Extrapolation to a different number requires only minor nomenclature changes. (See 'Nomenclature' chapter for variables meaning)

The component mass balances for each spherical sector are given by:

$$\frac{dm_{j,i}}{dt} = J_{j-1,i} - J_{j,i} + R_{j,i} \qquad (1)$$

where $R_{j,i}$ [kg/s] is the production rate due to chemical reactions. The mass flux $J_{j,i}$ results from two different contributions:

$$\text{Diffusion} = -D_{j,i} \left.\frac{dC_{j,i}}{dr}\right|_{j=r_j} S_j \; por_j \qquad \text{Pression} = -y_{j,i} \frac{Da_j}{\mu_j} \left.\frac{dP_j}{dr}\right|_{j=r_j} \rho_j \; S_j por_j$$

At the external surface, the diffusion contribution is replaced by the flux exchanged with the bulk phase (analogously the pressure contribution takes into account of the bulk pressure): $\text{Diffusion} = U_i (C_{NR,i} - CB_i) S_{NR} \; por_{NR}$

The enthalpy balance around each sector *j* is mainly dependent on conduction and reactions duties:

$$\frac{d\sum_{i=1}^{NCP} m_{j,i} Cp_{j,i} T_j}{dt} = JC_{j-1} + \sum_{i=1}^{NCP} J_{j-1,i} h_{j-1,i} - JC_j - \sum_{i=1}^{NCP} J_{j,i} h_{j,i} + HR_j \qquad (2)$$

JC_j [kj/s] is the heat flux due to conduction exiting the sector *j*. At the external surface, JC_{NR} becomes the flux exchanged with the bulk phase.

HR_j [kj/s] is the total heat production rate in the sector ‘j’ due to chemical reactions. The mass component equations and enthalpy balance in the gas phase are:

$$\frac{dg_i}{dt} = G_{0,i} + J_{NR,i}\eta + R_{g,i} - G_i \tag{3}$$

$$\frac{d\sum_{i=1}^{NCP} g_i Cp_i Tg}{dt} = \sum_{i=1}^{NCP} G_{0,i} hg_{0,i} + \sum_{i=1}^{NCP} J_{NR,i} h_{NR,i}\eta + JC_{NR}\eta + HR_g - \sum_{i=1}^{NCP} G_i hg_i \tag{4}$$

where HR_g [kj/s] is the total heat production rate due to gas phase reactions, η is the total number of particles in the bed.

Finally ancillary equations are added to complete the model at hand:

- Continuity on total gas flowrate $\sum G_i = \sum (G_{0,i} + J_{NR,i}\eta)$
- Shrinking of particle sectors (solved for r_j)
  $$\frac{4}{3}\pi (r_j^3 - r_{j-1}^3)\, \rho_j^* (1.- por_j) = \sum_{i=1}^{NCP^*} m_{j,i}$$
  (NCP^* is the total solid and liquid components number, ρ_j^* is the density of such a mixture)
- Shrinking of the reactor bed (solved for Z) $A\,Z = \eta\, V_p /(1-\varepsilon)$
- Pressure inside each particle sector (solved for new P_j):
  $$P_j \frac{4}{3}\pi (r_j^3 - r_{j-1}^3)\, \rho_j^{**} por_j = \frac{R_{GAS}\, T_j}{M_{wj}} \sum_{i=1}^{NCP^{**}} m_{j,i}$$
  (NCP^{**} is the total gas components number, ρ_j^{**} is the density of such a mixture, M_{wj} is its molecular weight and R_{GAS} is the gas constant)

Dependence of the porosity and the bed void fraction on the particle morphology is here neglected. The model of the single element is constituted by a system of [(NCP+1)*NR + NCP+1] ODE equations (1-4), with the initial conditions at t=0. The ancillary equations form a disjoint system of algebraic equations that is sequentially solved at each integration step. The large ODE system has been solved by using BzzMath library, which is available on the Internet and is downloadable as freeware software for non-commercial use from www.chem.polimi.it/homes/gbuzzi/

3.2. Moving Bed Model

The standard moving bed gasifier requires a ash continuous removal from the bottom to maintain the combustion zone in a relatively fixed vertical position and a top feed rate modulated to maintain a fixed top of bed level within the gasifier (Fig. 1. b). The particle discretization is the same of the one used in the previous batch model description. Again for sake of simplicity in exposition a single reactor bed element is assumed. The nomenclature adopted by the fixed bed model is valid also in this description. The extent of the bottom extraction depends case to case from several controlling variables including the concentration reached on the bottom by inert components. For sake of example let suppose the following simple relation:

$$S = \frac{x_{ash} - x_0}{1.- x_0} S_m$$

where S [kg/s] is the extraction rate, x_{ash} is the actual ash mass fraction, x_0 is its initial value equal to that one in the top feed and S_m stands for the maximum expected value of S. The extraction rate S may be rewritten as the product $N*m_p$, where N is the number of particle extracted per second and m_p the mass of a single particle. N_0 and m_{p0} will denote the same quantities in the top feed. Assuming that both the particle porosity and the bed void fraction are constant along the time, the constant reactor volume (Vr) is obtained by imposing the following condition:

$$\frac{dVr}{dt} = \frac{N_0 m_{p0}}{\rho_0} + \eta \sum_{j=1}^{NR} \frac{1}{\rho_j} \sum_{i=1}^{NCP} \frac{dm_{j,i}}{dt} - \frac{Nm_p}{\rho} = 0 \qquad (5)$$

The hold-up η (number of particle in the bed) changes in the time according to:

$$\frac{d\eta}{dt} = N_0 - N \qquad (6)$$

The integration of (6) allows obtaining the desired value of N_0 from the algebraic equation (5).

The balance equations governing the whole process are directly derived from those ones already presented for the fixed bed model with slight modifications.

$$\frac{dm_{j,i}}{dt} = J_{j-1,i} - J_{j,i} + R_{j,i} + N_0 m_{0\,j,i} - Nm_{j,i} \qquad (7)$$

$$\frac{d\sum_{i=1}^{NCP} m_{j,i} Cp_{j,i} T_j}{dt} = JC_{j-1} + \sum_{i=1}^{NCP} J_{j-1,i} h_{j-1,i} - JC_j - \sum_{i=1}^{NCP} J_{j,i} h_{j,i} + HR_j + \sum_{i=1}^{NCP} (N_0 m_{0\,j,i} h_{0i} - Nm_{j,i} h_{j,i}) \qquad (8)$$

It is reasonably acceptable that the gas phase may be described by the previous equations (3) and (4), due to the limited entrainment of gas into the solid feed. The system of equations 3-8 when solved simultaneously provides the desired process description.

3.3. Drop Tube Model

For sake of kinetic modeling studies of gasification and combustion of biomasses, many experiments are conducted inside entrained flow or drop-tube reactors (Fig. 1. c). Gas and particles are continuously fed at the top of the tube through two different nozzles. Gas enters at temperature, mass flowrate and velocity usually higher than the solid particles. Steady conditions are easily reached by the system and this allows to make all the desired experiments.

Again with the same previous particle discretization and nomenclature, the steady conditions of this system are described along the reactor height.

Contact time of solid particles is given by the definition of the particle velocitys derived from momentum equation:

$$m_p \frac{dv_p}{dt} = -(\rho_p - \rho_g)\, a\, V_p \sin(\alpha) - 0.5\, f\, \rho_g (v_p - v_g) \left| (v_p - v_g) \right| \qquad (9)$$

where v_g [m/s] is the gas spatial velocity, a [m/s^2] is the gravity, α[deg] is the inclination of the reactor vs. horizontal line; *f* is the friction factor depending on Reynolds number. The particle behavior is described by the equations (1) (2) adopted in the fixed bed model. The mass gas component equations are:

$$\frac{dwg_i}{dt} = v_p A\, (J_{NR,i}\eta + P_{g,i}) \qquad (10)$$

where η indicates the number of particles per m^3 of reactor (η_0 at reactor inlet), $J_{NR,i}\eta$ [kg/m^3 s] is the total mass exchanged by the gas phase with the particles.

The gas enthalpy balance is:

$$\frac{d\sum_{i=1}^{NCP} wg_i Cp_i T_g}{dt} = v_p A\, \Big(\sum_{i=1}^{NCP} (J_{NR,i} h_{NR,i})\eta + JC_{NR}\eta + HR_g\Big) \qquad (11)$$

HR_g [kj/m^3 s] is the total heat production rate due to gas phase reactions

Two further ancillary equations, continuity on total particle number and on total gas flowrate, are added to complete the model.

4. Example

Biomass is pyrolysed under high temperatures and flash heating rates conditions in a drop tube reactor. Particles of 0.4 mm diameter are fed to the reactor and the gas released is more than 70 wt % of the initial weight. The particle residence time is about 1 s while the gas residence time is about 3.5 s. The equivalent initial composition of the biomass $C_6H_{8.8}O_{3.9}$ becomes $C_6H_{2.9}O_{1.1}$ at 1073K and $C_6H_{1.4}O_{0.5}$ at 1273K, at the reactor outlet. These results are in good agreement with the experimental measurements indicating a composition of $C_6H_{2.7}O_{0.8}$ and $C_6H_{1.5}O_{0.4}$, respectively. The predicted char yield is ~14 wt% of the initial dry biomass, in a very good agreement with the experimental measurements.Experimental (Dupont et al. 2007) and predicted results are compared in Fig. 2. CO is the major species in both model and experiments, followed by H_2 and H_2O. There is a good agreement on CO_2, which is present only in small amounts. *Tar* species decompose in the gas phase and significantly contribute to the formation of methane, acetylene, ethylene and heavier hydrocarbons. While acetylene and ethylene predictions agree with the experimental measurements, methane predictions are underestimated by the model. The temperature effect on CO and H_2 is not very sensible because the devolatilization process is practically completed even at 1073 K. On the contrary, it is possible to observe that the model properly predicts the different trends of ethylene and acetylene. In fact, C_2H_2 is more abundant than C_2H_4 at high temperature, while the reverse behavior is predicted and measured at 1073 K.

The results of Fig. 2 clearly indicate not only the possibility of the model to correctly predict the amount and composition of the solid residue, but also show the importance of the successive decomposition of the released products.

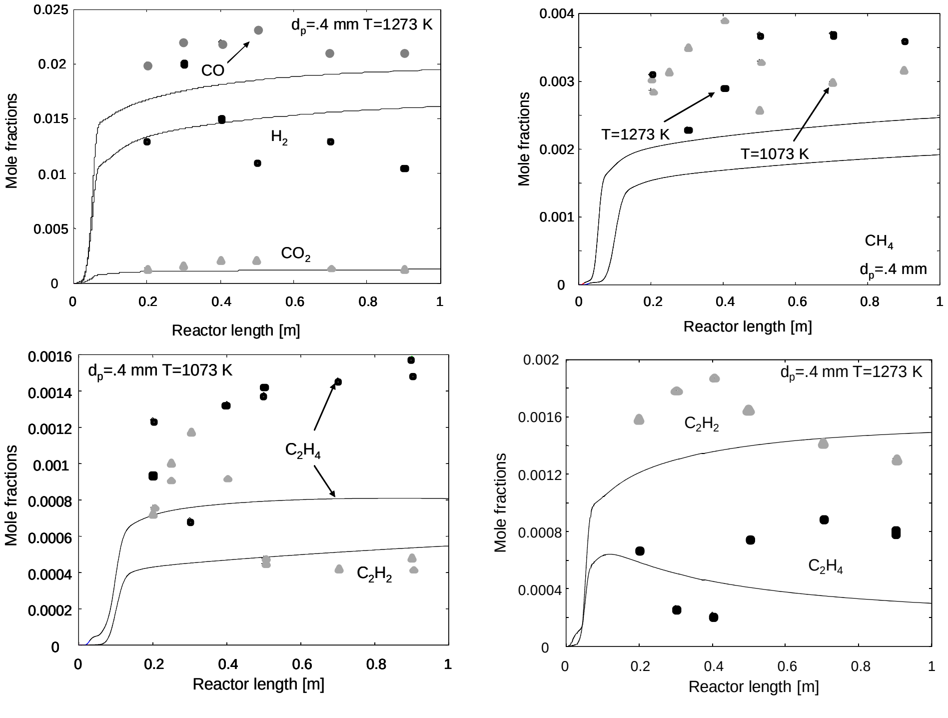

Fig. 2. Comparisons between experimental data (points) and model predictions (lines) at 1073 K and 1273 K for 0.4 mm particles

As far as the kinetics of gasification and combustion of char residue is concerned, it is assumed that only the final char residue is reactive and usual kinetic laws of pure carbon are used.

Nomenclature

A	[m^2]	reactor cross section
CB_i	[kg/m^3]	gas bulk concentration of component *i*
$C_{j,i}$	[kg/ m^3]	gas concentration of component *i* in the sector *j*
$Cp_{j,i}$	[kj/ kg K]	heat capacity of component *i* in the sector *j*
Da_j	[m^2]	Darcy coefficient in the sector *j*
$D_{j,i}$	[m^2/s]	effective diffusivity of component *i* in the sector *j*
g_i	[kg]	mass of component *i* in the gas phase
G_i	[kg/s]	flowrate of *i* in the gas at bed exit (G_{0i} at bed inlet)
$h_{j,i}$	[kj/ kg]	specific enthalpy of component *i* in the sector *j*
hg_i	[kj/kg]	specific enthalpy of component *i* in gas phase (hg_{0i} at bed inlet)
$J_{j,i}$	[kg/s]	mass flux of component *i* exiting the sector *j*
$m_{j,i}$	[kg]	mass of component *i* in the sector *j* (m_p is the total mass)
$P_{g,i}$	[kg/m^3 s]	total mass production rate due to gas phase reactions
Por_j	[m^3/m^3]	particle porosity (pore volumes / total volume of sector *j*)
$R_{g,i}$	[kg/s]	total mass production of component *i* due to gas phase reactions
T_g	[K]	Temperature in the gas phase
V_p	[m^3]	particle volume
$y_{j,i}$		gas mass fractions
wg_i	[kg/s]	gas flowrate of component *i* ($wg_{i,0}$ at the bed inlet)
Z	[m]	reactor height
λ_j	[kj/mKs]	thermal conductivity of sector *j*
η		number of particles in the reactor bed
ε	[m^3/m^3]	bed void fraction
μ , μ_j	[kg/m s]	gas viscosity and gas viscosity in the sector *j*
ρ_g , ρ_j	[kg/m^3]	gas density and gas density in the sector *j*
ρ_p	[kg/m^3]	density of the particle

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