

Mathematical modelling of gasification and combustion of solid fuels and wastes

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Gasification of solid fuels is nowadays a promising alternative to direct combustion. This work presents a general mathematical model of gasification and combustion units where both the transport resistances and the chemical kinetics are important at the particle scale. Pyrolysis and devolatilization of the solid fuel is only the first step of the entire process. Successive gas phase reactions of the released species require both a proper description of the gas-solid transport equations as well as the characterization of gas-solid combustion and gasification reactions.

At the reactor scale the numerical complexity of the resulting problem derives first of all from the large number of involved species and reactions and also from the stiff nature of the overall system. A couple of examples relating to coal combustion and biomass gasification allows the evaluate the possibility and limitations of the proposed approach.

1. Introduction

The environmental concerns towards the combustion of fossil fuels drive the interest in gasification processes of biomasses, plastics, wastes and refuse derived fuels (RDF). The need of mathematical models for the optimal design and operation of these industrial units is well recognized [Di Blasi, 2008], both for fuel devolatilization and for the successive gas phase reactions. Multistep kinetic models of plastics and biomass pyrolysis, as well as pyrolysis and combustion reactions in the gas phase were already discussed elsewhere [Faravelli et al., 2001, Ranzi et al., 2001 and 2008].

2. Devolatilization of Coals, Plastics and Biomasses

2.1 Coals

A multistep kinetic model has been recently developed [Sommariva et al., 2009]. This model refers and represents the actual coal in terms of a linear combination of three reference coals (lignitic, bituminous and anthracitic) and gives detailed information on the residual char as well as on the speciation of released gas and tar components. Fig. 1 shows a sample of comparisons between model predictions and experimental data obtained by Xu and Tomita [1987]. Xu and Tomita [1987] analysed the devolatilization of different coals with a carbon content varying from 65 % (lignite) up to 94 %

(anthracite) in a Curie point pyrolyzer, with heating rate of ~ 3000 K/s, final temperatures up to 1193 K and end-time of 4 s.

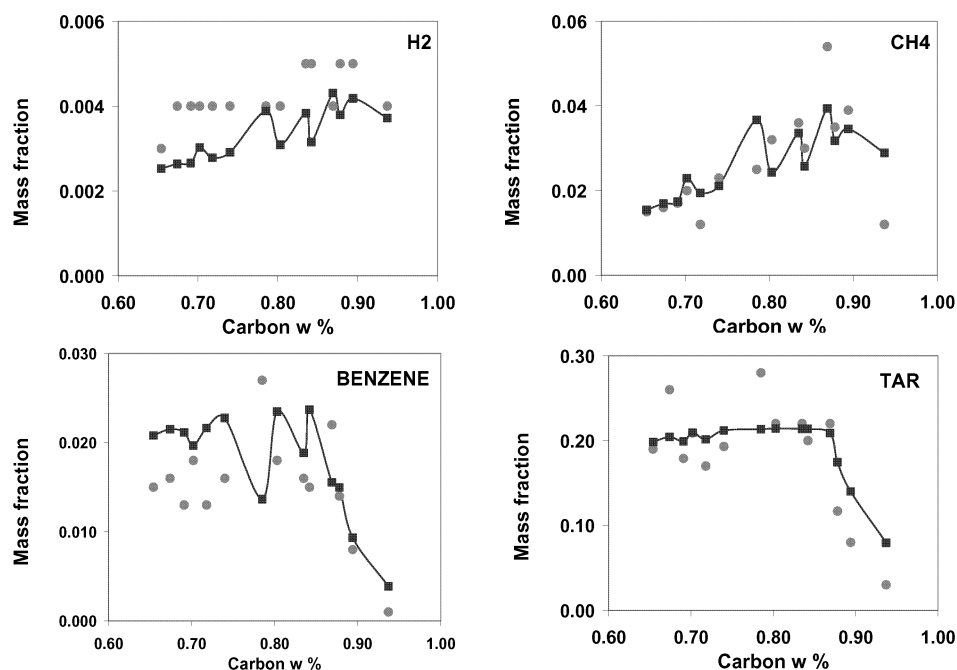


Figure 1: Comparisons between model predictions (lines) and experimental results (points) [Xu and Tomita, 1987].

2.2 Plastics

Devolatilization models of main plastic wastes, such as poly-ethylene (PE), poly-propylene, polystyrene (PS) and poly-vinyl-chloride were already discussed in a previous paper [Marongiu et al., 2007]. Fig.2 shows a sample of typical degradation curves for the four different polymers.

2.3 Biomasses

As in the case of coals, biomass devolatilization is considered a straightforward combination of the pyrolysis of three reference components: cellulose, hemicellulose and lignin. Although extractives, either soluble in water or in organic solvents, usually account for less than 10% of the total biomass, they are ignored as participating to biomass characterization. Predictions from these models reproduce correctly the experimental thermo gravimetric (TG) curves during the pyrolysis of several biomasses. [Ranzi et al., 2008]. As a simple example, Table 1 reports the multistep kinetic model assumed for cellulose decomposition.

Table 1: Multistep kinetics of cellulose devolatilization

	$k [s^{-1}], \text{ kmol}, \text{ m}^3, \text{ K}$
CELL > CELLA	$8 \times 10^{13} \exp(-46000/RT)$
CELLA > $0.95 \text{ C}_2\text{H}_4\text{O}_2 + 0.25 \text{ C}_2\text{H}_2\text{O}_2 + 0.2 \text{ CH}_3\text{CHO} +$ $0.25 \text{ C}_6\text{H}_6\text{O}_3 + 0.2 \text{ C}_3\text{H}_6\text{O} + 0.2 \text{ CO}_2 + 0.15 \text{ CO} + 0.1 \text{ CH}_4$ $+ 0.9 \text{ H}_2\text{O} + 0.65 \text{ CHAR}$	$10^9 \exp(-30000/RT)$
CELLA > $\text{C}_6\text{H}_{10}\text{O}_5$	$4 \times T \times \exp(-10000/RT)$
CELL > $5.0 \text{ H}_2\text{O} + 6.0 \text{ CHAR}$	$8 \times 10^7 \exp(-32000/RT)$

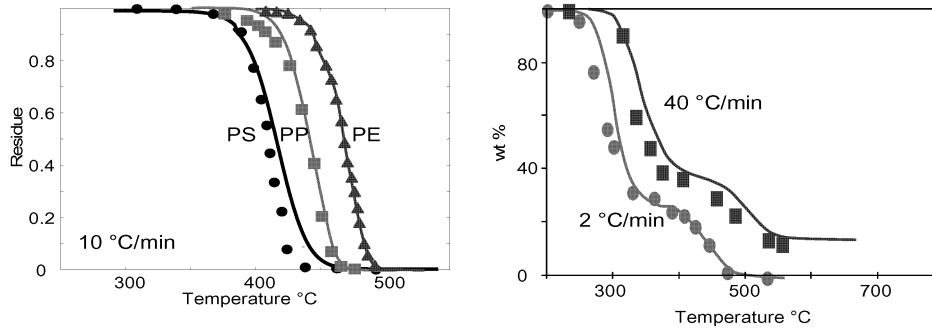


Figure 2. Comparison of plastic degradation model with experimental data a) PE, PP and PS pyrolysis; b) PVC pyrolysis .

3. Combustion and gasification reactions of residual char

The gasification and combustion of char, i.e. the set of heterogeneous reactions of oxygen and steam with the solid residue coming either from coal, biomass or plastics are responsible for the autothermic behaviour of the whole gasification process. They are summarized in Table 2.

Table 2: Char Gasification and Combustion Reactions

	$\text{ kmol}, \text{ m}^3, \text{ K}, \text{ s}$
$\text{CHAR} + \text{O}_2 > \text{CO}_2$	$5.7 \times 10^9 \exp(-38200/RT) [\text{O}_2]^{0.78}$
$\text{CHAR} + 0.5 \text{O}_2 > \text{CO}$	$5.7 \times 10^{11} \exp(-55000/RT) [\text{O}_2]^{0.78}$
$\text{CHAR} + \text{H}_2\text{O} > \text{CO} + \text{H}_2$	$7.9 \times 10^9 \exp(-52000/RT) [\text{H}_2\text{O}]^{0.7}$

4. Gas-solid interactions

The numerical approach adopted in this work focuses the attention not only on the description of the chemistry of solid fuel devolatilization, but also on mass and heat transfer processes at the particle and reactor scales. In particular, two main sub-models,

which will be briefly described in this section, are properly combined to obtain a global mathematical model describing a number of reactor typologies.

4.1 Particle scale

The solid fuel particle, which consists of a mixture of reference components and possibly ash, is assumed as a homogeneous sphere with NS internal sectors, that account for possible heat and mass transfer resistances. Particles release gases to the surrounding gas phase, while surrounding gases diffuse into the solid particle. A simplified scheme of the elemental gas-particle module indicating the gas-solid interactions and the release of components is reported in Figure 3. The balance equations of mass species and energy can be found elsewhere [Dupont et al., 2009].

Released components can either mix with the surrounding gases or, at lower temperatures, can condensate on cold surfaces. Gas phase is considered as a perfectly stirred reactor inside the cell module. Convective fluxes or flow rates entering and exiting the module are allowed, both for gas and solid phase. The C++ BzzDAE solver is used to numerically handle this mathematical model. Physical and mathematical details on the overall complexity of this problem are given elsewhere [Buzzi and Manca, 1998].

4.2 Reactor scale

The elemental module described above is flexible and suitable for simulating different process alternatives, such as fixed or moving bed gasifiers and combustors, updraft or downdraft configurations and also the entrained flow reactor. Figure 3 shows some of these examples. In particular, the entrained flow reactor model is extensively described in [Dupont et al., 2009]. On the contrary, additional references about the equations governing the biomass gasifier model discussed in the next section can be found in [Pierucci and Ranzi, 2008].

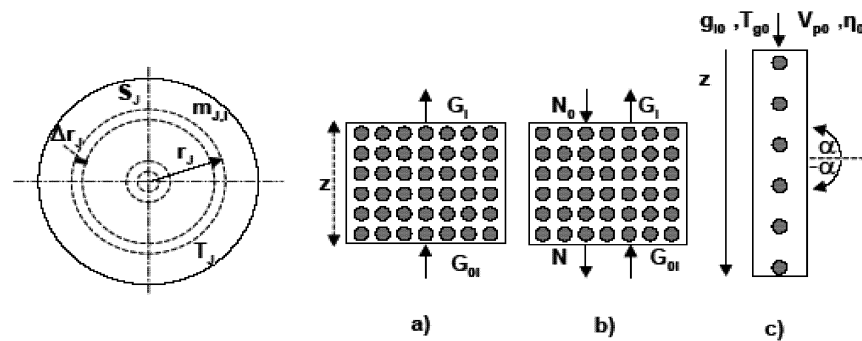


Figure 3. Scheme of the elemental gas-particle module and of several gas-solid configurations: a) fixed bed reactor; b) counterflow reactor; c) entrained flow reactor.

5. Successive gas phase reactions

Volatile components released from coals, plastics and biomasses are subject to successive decomposition and oxidation reactions in the gas phase. Hydrocarbon species released from plastics and tar species released from coals are already considered

in a general and detailed kinetic scheme of pyrolysis and oxidation of hydrocarbons [Ranzi et al., 2001]. Similarly, the primary propagation reactions of oxygenated species released from biomasses form intermediate products still considered in the previous kinetic scheme. The whole kinetic scheme together with thermodynamic properties of all involved species are available in CHEMKIN format on the web site [<http://www.chem.polimi.it/CRECKModeling/>]

6. Application Examples

Two different examples are briefly discussed in this paper. The former relates to high temperature coal combustion in an entrained flow reactor, while the latter illustrates some preliminary results of a fixed bed biomass gasifier.

6.1 High temperature coal combustion in an entrained flow reactor.

Pulverized coal is here burned at high temperature in a vertical drop-tube furnace under two different gas mixtures (O_2/N_2 and O_2/CO_2) at different O_2 partial pressures. The temperature–time profiles are investigated to study the effect of replacing N_2 with CO_2 on particle combustion. Figure 4 shows model predictions for bituminous coal particles (45–180 μm). Coal temperature reaches ~ 2200 K in the O_2/N_2 system, while lower temperatures are reached when replacing N_2 with CO_2 , due to the different heat capacity. These values well agree with experimental measurements. Figure 4 also shows the predicted and observed burnout times of the bituminous coal both in O_2/N_2 and in O_2/CO_2 . Model predictions are close to the average experimental values, but model cannot distinguish between the two systems. Temperatures are large enough and, as expected, a mass transfer regime is observed, without apparent influence of the temperature. The effect of CO_2 gasification reaction could not contribute to explain this aspect and a further analysis with careful estimation of transport properties is required.

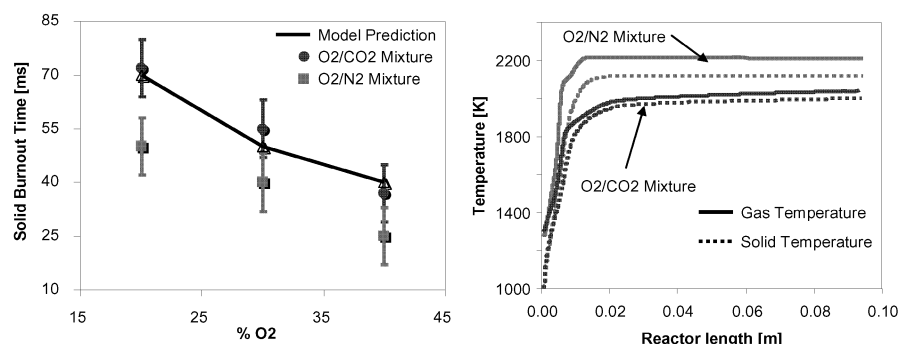


Figure 4: Coal particle burnout [Bejarano and Levendis, 2008]

6.2 Biomass gasification

Figure 5 shows the predicted results of a counter-current fixed bed gasifier of biomass. Cellulose particles of 1 cm are treated with air at stoichiometry ratio 0.33. When air and solid flowrates increase the gasification process is incomplete, fuel particles leave the unit at high temperature and ashes still contain unconverted material. The model characterizes the solid and gaseous streams including a large detail of unconverted tar components and becomes an useful tool for the design of gasifier units.

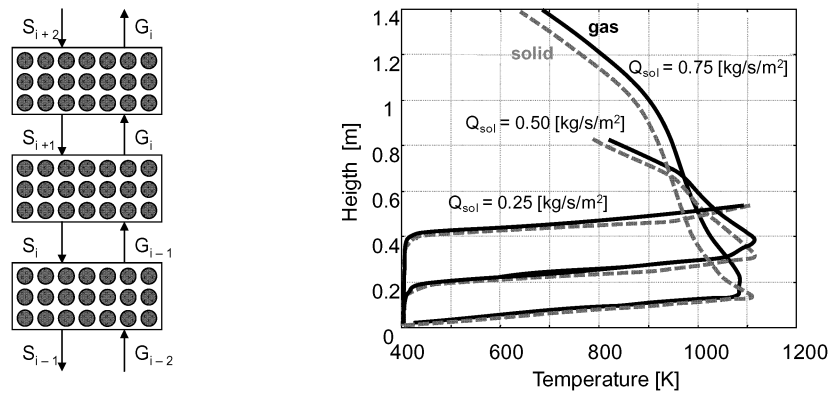


Figure 5: Counter-current fixed bed biomass gasifier. Vertical Temperature profile of gas (solid lines) and solid phase (dotted lines).

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