



A kinetic approach to the mathematical model of fixed bed gasifiers

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ABSTRACT

This work presents a comprehensive mathematical model of a fixed bed gasifier, where heat and mass transport resistances and chemical kinetics are accounted for both at the reactor and the particle scale. A multistep kinetic model of devolatilization of solid fuels, such as coals, plastics, biomasses and wastes has been employed and validated. The kinetic model of refuse derived fuels (RDF) and wastes is simply based on a linear combination of the devolatilization models of its main constituents. Ligno-cellulosic and plastic materials, together with ash and moisture, allow to account for the high heterogeneity of RDF. Successive gas phase reactions of the released species are described with a detailed kinetic scheme. Furthermore, an accurate description of heat and mass transport between gas and solid phases allows the proper characterization of combustion and gasification of the solid fuel at the particle and reactor scale. The mathematical model of a counterflow fixed bed reactor is then applied first to discuss the importance of heat transfer resistances at the particle scale, then to describe coal and biomass gasification. This work summarizes several facets of this problem with validations and examples and it allows to evaluate feasibility and limitations of the proposed approach.

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1. Introduction

The environmental apprehension towards the combustion of fossil fuels together with the growing concern on waste materials drive the interest in gasification processes of biomasses, coals, plastics, and refuse derived fuels (RDF). Pyrolysis and gasification of solid fuels are nowadays promising alternative to direct combustion, both electric and thermal energy are viable products, together with chemicals. Gasification is a robust proven technology that can be operated either as a simple, low technology system based on a fixed-bed gasifier, or as a more sophisticated system using fluidized-bed technology (McKendry, 2002). The properties of the biomass feedstock and its preparation are key design parameters when selecting the gasifier system. Differences between fixed bed and fluidized bed gasifiers are discussed by Warnecke (2000). The mathematical description of such processes is rather difficult due to the complex phenomena involved, such as modelling solid devolatilization, gas–solid interactions and secondary gas phase reactions.

During last years, many efforts have been devoted to understand and describe gasification process (Biagini, Masoni, Pannocchia, & Tognotti, 2009; Recman & Hájek, 2009; Juřena, Recman, & Hájek, 2009). Gronli and Melaen (2000) studied wood pyrolysis using a mono-dimensional model, devoting a particular attention both

to kinetics and transport resistances inside the biomass particles. Thunman and Leckner (2005) explored the influence of particle size and fuel density during oxidation process in a fixed bed reactor. In particular they showed that inter- and intra-particle resistances, more important in bigger particles, lead to different temperatures inside the particles and between solid surface and gas phase. Also Yang, Ponzio, Lucas, and Blasiak (2006) analyzed the importance of chemical and physical processes during gasification showing the influence of oxygen concentration, fuel ratio and process temperature. Di Blasi (2004) developed a comprehensive model able to describe wood gasification in a counter current flow reactor. Such a model is able to describe the dynamic behaviour of the system taking into account mass and thermal diffusion along the reactor. The density of the bed varies in the devolatilization region, while solid velocity is assumed constant. On the other side, during gasification and combustion solid velocity changes due to the reaction effect, while bed density remains constant. A one-dimensional model of countercurrent fixed-bed coal gasification has been developed and discussed by Hobbs, Radulovic, and Smoot (1993). Solid velocity is there evaluated using continuity equation, bed density is kept constant and porosity varies with conversion. Finally, Corella, Toledo, and Molina (2007) analyzed the economic feasibility of different biomass gasification processes.

It is then clear that this multiscale and multiphase problem does require a very careful attention in order to define and develop at least preliminary models. However, it is worth to emphasize the importance of these models, which could first improve the understanding of the whole process and then simplify the scale-up and

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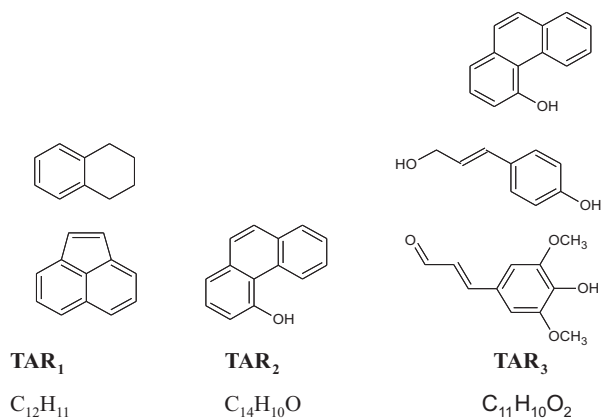


Fig. 1. Lumped reference components of tar products from reference coals.

the optimization of the gasifier. In this work, we proposed the methodology for solving such problems, showing the approach for the main facets involved in solid fuels gasification. Finally, an application example of a fixed bed gasifier model is provided, emphasising the thermal features of the reactor as well as the role of feedstock characterization.

2. Devolatilization of coals, plastics, biomasses and refused derived fuels (RDF)

2.1. Solid fuel characterization

The different solid fuels are described with a limited number of reference compounds and for each of them a multistep kinetic scheme was developed. While plastics, such as poly-ethylene (PE), poly-propylene (PP) and poly-styrene (PS) have a very well-defined structure and composition, the available information about coals and biomasses is usually limited to the elemental composition in terms of C/H/O. Degradation of plastics was already discussed by Marongiu, Faravelli, and Ranzi (2007). On the contrary biomass and coal have less defined and regular structures and they require a more empirical approach or better they do require further simplifications and a more careful discussion.

Biomass composition, if biochemical analysis is available, is simply defined in terms of humidity, ash, cellulose, hemicelluloses and lignin. If only the elemental analysis is available, then a suitable combination in terms of reference species is derived by atomic balance (Ranzi et al., 2008). Several applications, mainly concerning thermo-gravimetric analysis are there reported, while further validation examples relating bio-oil formation are reported in Calonaci et al. (2010). Finally, syngas production from biomass gasification in an entrained flow reactor at high temperature is discussed in Dupont et al. (2009).

Following a very similar approach, the composition and reactivity of the different coals are described by using three reference species (COAL₁, COAL₂ and COAL₃). COAL₁ (C₁₂H₁₁), together with pure carbon (CHARC), is useful to describe anthracitic coals with different degree of aromaticity. COAL₂ (C₁₄H₁₀O) lies in the middle of bituminous coals, while COAL₃ is highly oxygenated (C₁₂H₁₂O₅) and is representative of lignitic coals (Sommariva, Maffei, Migliavacca, Faravelli, & Ranzi, 2010).

Thus, the novelty of this kinetic model, when compared with the majority of the available ones in the literature, is the effort to describe the devolatilization reactions with a lumped characterization of gas and tar released. Thus, Fig. 1 shows the lumped reference components describing the primary tar species released by coal devolatilization. Operating conditions affect the devolatilization selectivity and yields; furthermore this multistep

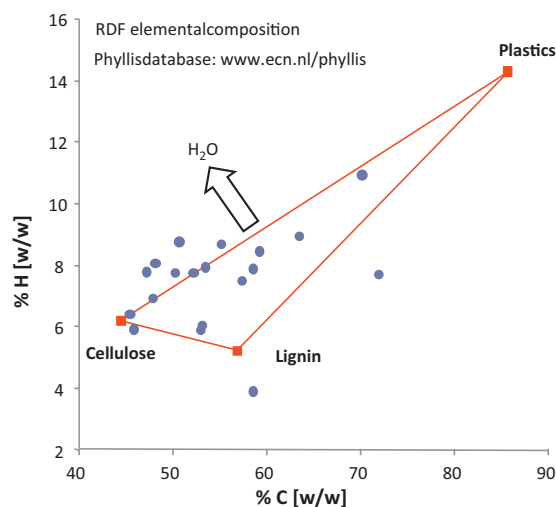


Fig. 2. Typical compositions of different RDF in terms of C and H (wt% ash free).

kinetic model allows also to describe the chemical and morphological evolution of the solid phase in terms of composition and reactivity.

In a very similar way, waste material and Refused Derived Fuels (RDF), typically with heating values of 4500–5000 kcal/kg, are described in terms of a proper combination of plastic wastes (15–30%), lignocellulosic material (30–50%), ash, and humidity (Giugliano, Grosso, & Rigamonti, 2008). Fig. 2 shows typical compositions of different RDF in terms of C and H (wt% ash free).

2.2. Solid fuel devolatilization

The RDF or the solid fuel particles are assumed as fixed mixtures of reference components. The overall kinetic model of devolatilization is simply the proper combination of the multistep devolatilization models of Biomass (Ranzi et al., 2008), plastic (Marongiu et al., 2007) and coal (Sommariva, Maffei, Migliavacca, Faravelli, & Ranzi, 2010). The peculiarity of this approach is that all these schemes consist of a limited number of devolatilization reactions, which are able to describe not only the solid residue, but also the detailed composition of released gas and tar species.

As already mentioned, approximate and elemental analysis allow to characterize RDF in terms of lingo-cellulosic species, plastics, ash and moisture. Buah, Cunliffe, and Williams (2007) reported interesting TG data and they showed that the selection of particle size used needs a particular attention, due to the variability of product yields depending on particle size. These differences could be attributed mainly at a different RDF composition, even if also intra-particle resistances, which strong depend on particle shape, could play a definite role.

Fig. 3 shows the weight loss curves of RDF particles of two different sizes versus temperature during TG analysis at 10 K/min under nitrogen. Predicted curves are obtained by varying RDF composition for fine and coarse particles. Plastic content, responsible of the second devolatilization step at 400–500 °C, is higher in coarse particles, while ashes or inert materials are more abundant in fine particles.

This dependence of RDF composition on the particle size was also observed in terms of different heating value by Skodras et al. (2008). They analyzed two RDF samples (RDF1 and RDF2) from different locations and processes with different elemental composition and heating values (Table 1).

While Skodras expect about 30% of plastic materials, only 25% of plastic material in RDF1 allows explaining both the larger heating value of this sample and the second step in the TG curve of Fig. 4a.

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