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Mathematical Modelling of Grate Combustion: Bed and Freeboard Coupling Issues

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This paper is focused on issues related to coupling of a fuel bed model with the freeboard as one of methods to simulate solid fuel combustion in grate furnaces. There are several problems, that have to be dealt with, when applying the coupled methodology, however previously not discussed in detail in literature. Topics, that are addressed, include the way of coupling, especially placement and discretization properties of the interface between the two computational models within the overall furnace model. As the bed model plays key role in this modeling approach, capabilities of existing models are reviewed. The emphasis is put on those features and problems that are not sufficiently solved in order to yield general and reliable model. One of these features is prediction of release of minor biomass and municipal solid waste constituents such as K, Cl, S and heavy metal elements as they are closely related to pollutant emissions formation and deposition, corrosion and erosion problems.

1. Introduction

Computational Fluid Dynamics (CFD) has become a standard supporting tool for design and optimization of all kinds of solid fuels utilization systems including grate combustors. Grate-firing is a widely used technology in biomass and municipal solid waste combustion for heat and power production. A typical CFD model of a grate combustor consists of a grate with primary air inlets, freeboard with secondary (and possibly tertiary) air inlets and heat exchangers in radiation and convection shafts. One of the key issues in the modelling is the degree of approximation of processes that take place in a fuel layer on the grate. In-bed processes are initiated by incident radiation from the freeboard. As combustion proceeds in the fuel layer, various gaseous products leave the bed entering the freeboard, for which values of gas species concentrations, temperatures and mass fluxes have to be supplied as inlet boundary conditions. Therefore, there is a strong coupling between the two regions.

There are three different approaches to treat the coupling (Yin et al., 2008b). The most frequently used method is based on an experience and design of a real furnace. A grate is divided along its length into four sections (drying, pyrolysis, char oxidation and ash cooling zones), for each of which profiles of temperature, mass flux and concentrations of gas species are prescribed as they are either measured in a real unit or calculated from mass and energy balance of the fuel. The method is satisfactory in cases where the subject of investigation does not lie in the vicinity of the grate, but sufficiently downstream of the bed as e.g. in one of the authors' previous works (Hajek et al., 2012).

In the second approach, the bed is defined as a porous zone, which creates resistance to fluid flow and generates pressure drop. Various source terms due to drying, pyrolysis, char oxidation and additional governing equations for solid fuel variables such as solid species mass fractions and temperature are defined within the zone to fully describe processes inside the fuel bed. Solution of the equations is left to the CFD code during the overall solution procedure. The method has been successfully demonstrated e.g. in (Collazo et al., 2012). Compared to previous method, it is capable to predict combustion and processes inside the fuel bed, however at the cost of increased computational times.

The attention of researchers has recently been attracted to development of a stand-alone numerical model of bed combustion, which is based on the same principles as porous zone bed model. Coupling of the two

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separate computational models (i.e. bed and freeboard models) is realized by a common interface, by means of which data (heat and mass fluxes) are shared and interchanged iteratively until convergence is reached in both models. Despite the fact that bed models are based on the same physical principles, differences can be found not only in the description of physical and chemical parameters, but also in the set of governing equations being solved due to various modeling assumptions. The most remarkable differences regard dimensionality of bed models and the extent to which both inter- and intra-particle effects are resolved. Such details are reflected in the way of coupling the bed model with the freeboard. For example, although one-dimensional transient models are developed mostly in order to study combustion in an experimental furnace (e.g. Zhou et al., 2005), transient solutions can be mapped onto horizontal positions of the grate using the so called walking-column method as described by Gort (1995) (see Figure 1) and applied by Yin et al. (2008b) in a coupled simulation of biomass combustion. On the other hand, the intermediate step of transforming the transient solutions to corresponding spatial positions is not necessary, if two- or three-dimensional bed model is used as demonstrated e.g. in (Yu et al., 2010).

Perhaps the most comprehensive coupled simulation of grate combustion is presented in (Simsek et al., 2009), where the fuel bed consists of a large set of thermally-thin spherical particles. In such kind of a model, effects of movement of grate bars on fuel mixing can also be studied in detail as in (Peters et al., 2011). These models are, however, very computationally demanding, especially if each particle is solved to obtain inside distributions of temperature and species mass fractions as well as for other inter-particle phenomena such as radiation. Recently, there have been efforts to speed up simulations of particle-resolved beds either by simplifying the used methodology, so that a representative particle is chosen and solved in each control volume, while others in the control volume are assumed to have the same properties (Anca-Couce et al., 2013), or by modifying the particle sub-model and optimizing numerical algorithms as in (Ström et al., 2013).

Yin et al. (2008b) concluded that reliability of a CFD model of grate combustion depends mainly on the quality of mesh and raw input data including boundary conditions at the grate inlet. These can be calculated using the bed model. It was stressed, that a reliable bed model had yet to be developed to account for noncontinuous fuel feeding, effects of grate movement and in-bed instabilities (for instance channelling) on flow patterns. From practical point of view, it is also important to include in the bed model the formation of precursors of gas phase reactions taking place in the freeboard such as N-, S- or Cl-related reactions to be able to check the emission levels or take into account fouling and slagging of heat transfer surfaces. Furthermore, the technique of coupling should not pose much difficulty to become a practical method for engineering practice. This article discusses issues related to coupled simulations of grate combustion.

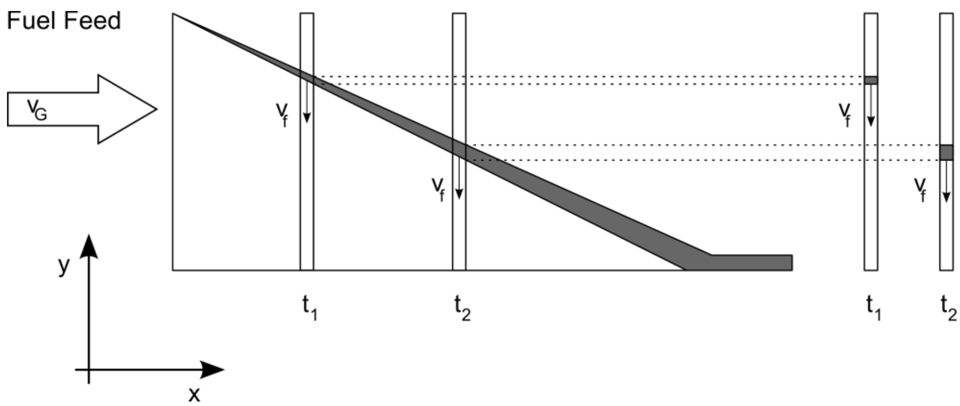

Figure 1: Walking column method. A fuel is moved on the grate with velocity v_G, so that horizontal position on the grate can be calculated using $\Delta x = v_G \Delta t$. As the combustion proceeds, the reaction front travels down with unknown velocity v_f.

2. Capabilities of bed models

It follows from the previous section, that numerous models of combustion in packed beds have been developed during the last two decades. It is not intended in this work to sort existing models into several classes. The purpose of this section is to provide information on capabilities of bed models and indicate topics and problems that are not solved to sufficient extent with respect to coupled-modelling methodology.

2.1 Heat and mass fluxes

The bed model is supposed to provide heat and mass fluxes for the freeboard model by solving relevant equations. As Yin et al. (2008a) pointed out, it is crucial to ensure, that the bed model is conservative, i.e. the model obeys essential physical principles such as conservation laws of mass and energy. Although a natural requirement it may seem, it is not precisely fulfilled in numerical simulations due to various sources of errors (Dahlquist, 1974). An imperfect conservation implies that the gas does not carry the right amount of mass and energy and therefore such a model cannot improve the estimate of boundary values at the inlet of a freeboard model.

While one-dimensional models can be verified directly by bench-top experiments, it is usually impossible to perform measurements in industrial combustion units in order to verify two- or three-dimensional bed models. Verification of these models can be based on the walking-column method as it was used e.g. in (Asthana et al., 2010). However, in lack of experimental data, conservativeness of the bed model can be examined theoretically by checking mass and energy balance of the model as e.g. in (Juřena et al., 2011).

2.2 Modelling of gas species formation

Biomass fuels are typically characterized by varying moisture content, higher volatile matter content and smaller amount of nitrogen (N) and sulphur (S) compared to coal. It is also interesting to note, that higher concentrations of N, S and chlorine (Cl) are usually found in herbaceous biomass (e.g. wheat straw, miscanthus, switchgrass, olive residues) than in woody biomass (e.g. spruce, willow, beech). The elemental composition of the fuel has impact, for example, on a level of emission formation (Obernberger et al., 2006).

During thermal conversion of the fuel, the solid matter is gradually decomposed and released as gaseous products. A set of gas species that are usually considered in simulations, is comprised of H_2O, O_2, N_2, H_2, CO, CO_2, CH_4, and tar, which is a complex mixture of condensable hydrocarbons and therefore, for simplicity, is usually represented by a single compound $C_xH_yO_z$. The chemical formula of tar can be deduced from mass and energy balance of the fuel. The major part of total gas volume is formed during pyrolysis. It is well known, that final yields of pyrolysis depend on a multitude of conditions including fuel type, its shape and size, local conditions under which it has been grown, heating rate and temperature. This is the reason, why there are large discrepancies in the reported kinetic and thermo-physical data describing pyrolysis. Yang et al. (2003) investigated the effect of various devolatilization rates on combustion parameters through a series of simulations and experiments. Variations in devolatilization rates were found to have significant effects e.g. on peak flame temperatures, concentrations of CO and H_2 at the bed top and ignition time, all of which play an important role in coupled simulations. Whether pyrolysis is considered to take place according to a global one-step reaction scheme as in most works on bed modelling (e.g. Zhou et al., 2005), or it is divided into several parallel primary reactions as in simulations of single particle pyrolysis (Haseli et al., 2011), care must be taken when defining the kinetic rates in any case.

Beside the afore-mentioned gas species that are commonly encountered in simulations, special case studies require description of formation of other species within the fuel bed as well in order to model all chemical reactions of interest in the freeboard. Modelling of NO_x has been included in a coupled simulation of straw combustion e.g. in (Yu et al., 2010), where fuel-nitrogen was assumed to be the main source of NO_x formation due to relatively low lower heating value of the biomass fuel. The intermediate specie which was formed during the pyrolysis stage as a precursor of NO_x was assumed to be NH_3.

Since slagging and fouling of heat transfer surfaces caused by ash deposition is a severe problem not only in straw-fired boilers, quite a lot of effort has been made to model and predict deposit formation on boiler walls as e.g. in (Kaer et al., 2006). This requires knowledge of mechanisms for prediction of release of alkali salts vapours within the fuel bed, mainly potassium chloride as the predominant stable alkali-bearing specie under combustion conditions, and kinetics of formation of sulphur dioxide. Although much experimental and theoretical work has been devoted to study of these mechanisms for various kinds of fuels (for instance, Peters et al. (2012) studied release of KCl and SO_2 from switchgrass, Johansen et al. (2013) investigated release of K, Cl and S from corn stover), comprehensive sensitivity analysis should be performed to check effects of various kinetic data and models on overall simulation results.

Modelling of release of heavy metals (Cd, Zn, Pb, Cr) during municipal solid waste incineration on a grate has also been attempted (Ménard et al., 2006), however, due to unavailability of data for description of kinetic evaporation rates, the predictions in the fuel bed were based on local themodynamic equilibrium calculations using minimization of the total Gibbs energy of a closed system.

2.3 Pressure drop

It is worth noting that very little attention is given in the published experimental works to the investigation of flow resistance in the fuel bed. This problem is rather pressing, because flow resistance of the bed in real combustors has decisive role in determining the local air-fuel ratio in the bed and thus influences all other processes through local heat generation rates. It has been either completely disregarded as in (Zhou et al., 2005) or a simple approximation assuming bed of spherical particles described by Ergun equation was adopted as in (Yang et al., 2007). The reason for adoption of such simplified approaches is the lack of experimental data both for model development and for its validation.

However, biomass particle shapes are far from being spherical. For instance, wheat straw particles are usually described as hollow cylinders. In spite of this fact, the Ergun equation with coefficients derived from measurements on spheres is still adopted for the description of local pressure drop in the bed of cylindrical particles, although it has been found inaccurate in case of a bed of non-equilateral cylinders (Foumeny et al., 1996). More attention should be paid to this issue both in experimental and modelling works.

A proper determination of pressure drop is also important from numerical point of view. While the top of the bed is treated as pressure outlet boundary condition in the bed model, pressure inlet boundary condition with the same value of pressure is specified at the grate inlet in the freeboard. Therefore, the inaccuracy of the pressure drop calculated across the bed is passed onto the freeboard as well.

3. Remarks on the coupling technique

In the coupled-modelling methodology, the fuel bed is physically separated from the freeboard, however, logically connected by the common interface, through which either of the models accepts data passed from the other one based on the current solution within the particular model. Transmitted data form dynamic boundary conditions for each model, so that solutions of both models are not independent of each other underlying the fact, that processes above the fuel bed are strongly influenced by, and therefore coupled to, in-bed processes and vice versa. However, physical separation of the two models has several implications.

3.1 Placement of the interface

One has to decide, where the freeboard model is cut off, i.e. where the interface is positioned. Since the bed profile along the grate is not known a priori, the interface cannot be defined as the top surface of the bed, which otherwise would become a natural choice. Two other options are on hand.

From a practical point of view, an optimal way of coupling the two models is to define the plane of a grate as the interface, where primary air properties entering the furnace are prescribed for boundary conditions in the experience-based modelling approach. Of course, it is an approximation of a real situation, since the part of the furnace volume occupied by a fuel layer is now left void allowing the flue gas species to react with the secondary combustion air closer to the grate.

The other option is to place the interface above the fuel layer, so that a part of the over-bed area is included in the bed model. This is applied in most of works on coupled simulation of grate combustion. In such arrangement, it must be ensured for the freeboard inlet boundary conditions that no back flows arise at the interface due to mixing of flue gases with secondary combustion air. Secondly, even though gas phase reactions are commonly included in the bed model within the fuel layer, the most part of the flue gas volume burns above the bed. Solution of the over-bed reactions can be left to the freeboard CFD solver, which may provide for more accurate and detailed chemical reaction schemes than the set of reactions defined in the bed model. Therefore, some loss of accuracy can be encountered, when placing the interface above the fuel layer, as a part of the over-bed area is solved within the bed model. However, this might not be significant depending on the local conditions.

3.2 Discretization properties

Following the walking-column approach (Figure 1), transient solutions of a one-dimensional model are related to corresponding positions on the grate (i.e. faces of the mesh) through the known velocity of the moving bed (grate) and a series of faces along the grate length represents a series of transient solutions of the bed model. Therefore, time steps in the bed model are determined from geometry and mesh properties of the grate such that

$$\Delta t = \frac{L}{vN} \text{ [s]} \tag{1}$$

where L [m] is the length of the interface, v [m/s] is the velocity of the moving bed and N [-] is the number of faces, that discretize the interface along its length. The time integration solver of the bed model should be robust to handle potentially long time steps depending on actual values of L, N and v. In certain cases, it might be necessary to divide the solution of a face into several (time) steps in order to obtain accurate temporal solutions. Of course, these considerations are irrelevant, if two- or three-dimensional bed model is used, as each face of the interface belongs to only and only one control volume in the bed model.

4. Conclusions

Three different approaches to modelling of grate combustion of solid fuels can be found in literature. They differ in the degree of approximation of processes occurring in the grate area, especially within the fuel bed. The most advanced method is based on separation of the combustion chamber into two zones – the bed zone and the freeboard region, and coupling them through boundary conditions at the common interface. The main feature of the method is that strong coupling of in-bed and over-bed processes is taken into account. This coupled-modelling methodology provides for deep insight into physical phenomena taking place both in the freeboard and bed regions depending on the degree of complexity of the bed model, which constitutes the key part of the overall model. The most comprehensive models treat the fuel layer as a large set of individual fuel particles allowing for studying the effects of grate bars motion on the particles, which is hard to achieve using other kinds of models. It is concluded that more attention should be paid to modelling of release of minor biomass or municipal solid waste constituents such as Cl, K, S and heavy metals in order to study their effect on combustion with respect to environmental aspects and operation of combustion units (slagging and fouling of heat transfer surfaces).

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