



Research article

Modeling of conversion of a single fuel particle in a CFD model for CFB combustion



Timo Niemi*, Sirpa Kallio

VTT Technical Research Centre of Finland Ltd, Kivimiehentie 3, Espoo, P.O.Box 1000, FI-02044 VTT, Finland

ABSTRACT

In CFD simulation of CFB combustion, computation of the local instantaneous conversion rate of a single fuel particle should be fast. Since fuel conversion is limited by mass and heat transfer and the rates of chemical reactions inside the particle, the optimal model would produce the internal conditions as a function of location. As rigorous 1D, 2D and 3D fuel conversion models presented in the literature are often too time-consuming for CFD environment, simplified 0D approaches have been suggested. To reduce the amount of simplification, the present study introduces an alternative approach that converts a rigorous fuel conversion model into correlations that can be implemented in a CFD code. As a demonstration example, a 1D shrinking particle model for coal combustion is converted into a correlation based description. The single particle model is used to produce a data set of net reaction rates averaged over particle volume in a wide range of fluidization, temperature and composition conditions. The data is then used to train neural network models that are fast to compute and easy to implement in a CFD code.

1. Introduction

For CFD simulation of a CFB furnace, computation of the conversion rate of a fuel particle should be fast to allow computing conversion of a large number of fuel particles at each time/iteration step. At the same time, the model should cover all the relevant chemical and physical phenomena. Mass and energy transfer rates in the particle and through the surrounding boundary layer and homogeneous and heterogeneous reaction rates are naturally the key factors determining the fuel conversion rates. However, modeling of these processes is complicated by the numerous chemical and physical phenomena that can simultaneously affect them. Depending on the conditions, drying, devolatilization and char conversion can occur in parallel, especially in large fuel particles [1]. During char combustion, gasification reactions have major importance on the conversion rate [2] especially in oxi-fuel combustion conditions [3]. Interaction has also been observed between the two gasification mechanisms with CO₂ and H₂O [4]. Changes in the porous structure and distribution of the ash during combustion affect the diffusion process, which leads to slowing down of the conversion [2] as combustion progresses. A transient modeling approach is required to model this effect [2,5]. Attrition of the surface layer of a particle is also important in fluidized bed combustion conditions [6,7] where typically ash is peeled off leaving no ash layer on the surface. Even the properties of the gas-particle suspension surrounding the

particle play a major role by contributing to the heat transfer rate [5].

Depending on the rates of mass transfer and reactions, the conversion process of a particle can be limited by the chemical reaction rates (leading to uniform conversion throughout the particle), the mass transfer rate through the boundary layer (reactions take place mainly at particle surface) or by a combination of diffusion and reaction rates. The last alternative is the typical mode of fuel conversion. It leads to concentration and temperature gradients inside the fuel particles, which need to be taken into account in modeling. To resolve the gradients, 1D modeling approaches that discretize particles into spherical elements have been developed [2,8]. Even more rigorous 2D and 3D models based on CFD [9,10] and discrete models based on percolation modeling in a cubic lattice of cells [11,12] have been suggested. These models can better take into account the 3D effects due to the flow field and/or the particle shape and internal pore structure.

In the case of simpler 1D [13] or 1.5D [14] furnace models, it is feasible to use comprehensive fuel particle submodels in which the chemical and physical processes occurring inside the particles are resolved in detail. For large-scale 3D CFD modeling of industrial CFBs, however, simplified approaches are needed to achieve sufficiently short computation times for the fuel particle submodels as most of the computational effort is required for the other parts of the simulation. Simplest modeling approaches suggested in the literature compute the oxidation rate from an Arrhenius expression accounting for kinetics,

* Corresponding author.

E-mail address: timo.niemi@vtt.fi (T. Niemi).

coupled with a model for oxygen diffusion through the boundary layer [15,16]. More accurate 0D models take into account also the incomplete penetration of the reactive gases by means of an effectiveness factor that is calculated with the Thiele modulus method [3,5,17,18]. Alternative approaches to model the boundary layer processes in the 0D description have been suggested [19].

Although the simplified models based on an effectiveness factors have proved to be acceptable in the case of combustion of a small spherical coal particle [5,17], they can significantly reduce prediction accuracy in other more complicated cases since they are based on several simplifications and assumptions. For example, taking into account particle shape, complicated interaction effects between the different reactions and non-uniform temperature distributions and porosity inside the particle is not possible with the simplified model structure. Thus, a more rigorous modeling approach could be of benefit to incorporate the available knowledge of fuel conversion processes in a form that can be used in CFD simulation of furnaces. For that purpose, the present paper suggests a modeling approach in which a correlation model is derived based on data produced with accurate physical models. In the paper, the approach is demonstrated by converting a fairly simple 1D shrinking particle model for coal combustion and gasification into a correlation based description that is fast to evaluate and can easily be implemented in a CFD code.

The shrinking particle model used as the basis in the work is the one of Konttinen et al. [20], augmented with expressions for gasification rates. In addition to the reactions taking place inside the particle, the shrinking particle model describes mass and heat transfer inside the particle and between the particle and the surrounding gas atmosphere. The model of Konttinen et al. includes also conversion of nitrogen species but in this work the methods are illustrated only for combustion and gasification reactions. In the study, the single particle model is used to produce net reaction rates averaged over particle volume in a wide range of fluidization, temperature and composition conditions. The goal of the study is to demonstrate the procedure for developing correlations that are fast to compute and easy to implement in a CFD code and simultaneously describe the single particle behavior with sufficient accuracy. Thus the focus of the paper is in the modeling procedure and not on the 1D model of char conversion. The paper discusses the possibilities to apply the same method using other more accurate fuel conversion models as the starting point.

2. Single particle modeling

The shrinking particle model used in the work describes the combustion of char-carbon and char-nitrogen in a spherical shrinking char particle. Ash is assumed to peel off from the surface as combustion progresses. For simplicity, homogeneous chemical reactions in the boundary layer are not accounted for. The model solves the equations describing reactions inside the particle and the diffusive transport of reactants inside and at the surface of the particle at a time instance assuming a pseudo-steady state. The results of the computation are the concentration and temperature profiles inside the particle and the transfer rates to/from the surrounding gas atmosphere. A detailed description of the model is given in Goel et al. [8], and in Konttinen et al. [20].

The governing material balance equation for single particle conversion is written as follows for component i inside the particle [8,20]:

$$D_{e,i} \left(\frac{\partial^2 c_i}{\partial r^2} + \frac{2}{r} \frac{\partial c_i}{\partial r} \right) + R_i(c_i) = 0 \quad (1)$$

where r is the radial position and R_i the local rate of the chemical reactions for component i : char-C oxidation and gasification and char-N oxidation and reduction. $D_{e,i}$ is the effective pore diffusion coefficient which is here assumed to be constant throughout a particle and also to be the same for all different gaseous species i . This is a severe

simplification since $D_{e,i}$ should depend on molecular mass of the gas species and pore properties that change as a function of char conversion fraction and location inside the particle. The change in pore area during char conversion also affects reaction rates. However, since the kinetic parameters used in the model were in Konttinen et al. [20] determined assuming constant $D_{e,i}$ and ignoring the effect of changing pore area and, moreover, Konttinen et al. [20] shows a good fit to the char conversion data of Tullin [21], the same simplifications were used here. To use a physically more realistic description for $D_{e,i}$ and pore area would have required re-estimation of the kinetic parameters which was considered unnecessary in this study that focuses on the procedure for converting a 1D single particle model to a correlation model usable in CFD.

Zero gradient is assumed as boundary condition in the middle of the particle and at particle surface the transport rates in the particle and between the particle and the surroundings are equal [8,22]:

$$D_{e,i} \frac{\partial c_i}{\partial r} \Big|_{r=r_p} = k_g (c_{i,\infty} - c_{i,s}) \quad (2)$$

where $c_{i,\infty}$ and $c_{i,s}$ are the concentrations of species i in the gas outside the boundary layer and at the surface, respectively. The external mass transfer coefficient k_g is calculated following the recommendations given by Palchonok [23]. A detailed presentation of the applied model is given by Konttinen et al. [20]. The models presented in Palchonok [23] were given for dilute and dense conditions and thus interpolation is performed in the code (see Konttinen et al. [20]).

For the calculation of the temperature, the following equations are applied (Konttinen et al. [20]):

$$\lambda_e \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) + \sum_{i=1}^{n_{het}} (R_i \Delta H_i) = 0 \quad (3)$$

$$\lambda_e \frac{\partial T}{\partial r} \Big|_{r=r_p} = \alpha_{tot} (T_\infty - T_s) \quad (4)$$

where λ_e is the effective thermal conductivity, ΔH_i is the reaction enthalpy of reaction i , and n_{het} is the number of reactions. α_{tot} is the net heat transfer coefficient given as the sum of particle convective, gas convective and radiative heat transfer contributions. The heat transfer coefficient is calculated according to the correlations given by Palchonok [23] for dense and dilute conditions and an interpolation in between [20].

The equations are solved using the finite-element code by Bergenwall [24]. The rates of the chemical reactions taking place inside the particles are calculated assuming the reaction mechanism for combustion and gasification and nitrogen chemistry. In the present study nitrogen chemistry is ignored and only carbon conversion is considered. The concentrations of nitrogen components, which are included in the Konttinen et al. [20] model, are in combustion conditions so small that they can be ignored while modeling the combustion and gasification rates. Reaction rates in the Konttinen et al. [20] model were determined for a bituminous coal and the reaction mechanism is shown in Fig. 1.

The single particle model computes the concentration and

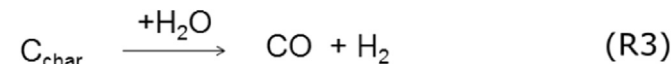
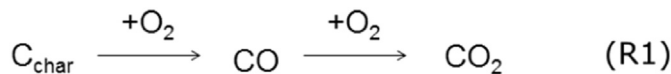


Fig. 1. The kinetic mechanism used in the single particle model.

Download English Version:

<https://daneshyari.com/en/article/4914335>

Download Persian Version:

<https://daneshyari.com/article/4914335>

[Daneshyari.com](https://daneshyari.com)