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

*Email: *timo.niemi@vtt.fi*

Abstract – In CFB combustion, fuel conversion is limited by mass and heat transfer and chemical reactions inside the particle. In CFD simulation, computation of the local instantaneous conversion rate of a single fuel particle should be fast. The objective of the present study is to convert a shrinking particle model for coal combustion into a correlation based description that can easily be implemented in a CFD code. The single particle model was used to produce net reaction rates averaged over particle volume in a wide range of fluidization, temperature and composition conditions. The data was used to train neural network models that are fast to compute and easy to implement in a CFD code.

INTRODUCTION

In CFB combustion, fuel particles are so large that fuel conversion is strongly limited by mass and heat transfer inside the particles. Thus particle size plays an important role and its effects should be accounted for in numerical modeling of CFB combustion. In the case of simpler 1D or 1.5D combustion models, it is feasible to use a detailed fuel particle model in which the chemical and physical processes occurring inside the particle are described as a function of the distance to the surface. In CFD simulation, however, computation of the conversion rate of a fuel particle should be fast to allow computing the conversion rates of a large number of fuel particles at each time/iteration step. The objective of the present study is to convert a shrinking particle model for coal combustion into a correlation based description that can easily be implemented in a CFD code.

The shrinking particle model used as the basis in the work was the one of Konttinen et al. (2002), 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 study 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 develop correlations that are fast to compute and easy to implement in a CFD code and simultaneously describe the single particle behavior with sufficient accuracy. The focus of the paper is in the modeling procedure.

SINGLE PARTICLE MODELING

The shrinking particle model describes the combustion of char-carbon and char-nitrogen in a spherical shrinking char particle. 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., (1994) and in Konttinen et al. (2002).

The governing material balance equation for single particle conversion is written as follows for component *i* inside the particle (Goel et al., 1994, Konttinen et al., 1999):

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

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. 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 (Goel et al., 1994, Konttinen et al., 1999):

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

where $c_{i,\infty}$ and $c_{i,s}$ are the concentrations of species i in the gas far of the particle and at the surface, respectively. The external mass transfer coefficient k_g is calculated following the recommendations given by Palchonok (1998). A detailed presentation of the applied model is given by Konttinen et al. (2002). The models presented in Palchonok (1998) were given for dilute and dense conditions and thus interpolation is performed in the code (see Konttinen et al., 2002).

For the calculation of the temperature the following equations are applied (Konttinen et al., 2002):

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

$$\lambda_e\left.\frac{\partial T}{\partial r}\right|_{r=r_p} = \alpha_{tot}(T_\infty - T_s) \tag{4}$$

where λ_e is the effective thermal conductivity, ΔH_i is the reaction enthalpy of reaction i, and n_{hetr} 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. It is calculated according to the correlations given by Palchonok (1998) for dense and dilute conditions and an interpolation in between (Konttinen et al., 2002).

The equations are solved using the finite-element code by Bergenwall (2000). 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. (2002) 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. (2002) model were given for a bituminous coal. The reaction mechanism is shown in Figure 1.

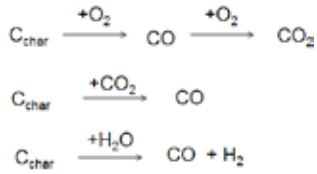

Fig. 1. The kinetic mechanism.

As results of the above integration, the rates of the reactions presented in Fig. 1 are obtained and the net formation/consumption rates of CO, CO_2, O_2, H_2O, and H_2 can be calculated.

DATA GENERATION AND ANALYSIS

In the study, the single particle model was used to produce net reaction rates averaged over particle volume in a wide range of conditions. As a first step, data was produced by varying each of the potential model inputs in a set of typical fluidized bed combustion conditions to evaluate its effect on the conversion rates. The variables considered were the concentrations of gas components and the temperature in the bulk gas, fuel particle diameter, and the variables required to describe heat and mass transfer to the surrounding gas: slip velocity between the particle and the gas, bed particle size and material density, and voidage. The effects of each of these variables were numerically evaluated in various CFB furnace conditions to find out whether in some conditions a parameter becomes important. As an example, Figure 2 shows the effects of some of the parameters on oxidation rates in typical low oxygen conditions at furnace bottom with O_2 concentration of 0.25 mol/m^3, H_2O concentration of 0.9 mol/m^3, CO_2 concentration of 1.4 mol/m^3, temperature of 1123 K and fuel particle diameter of 0.8 mm, when each of the parameters was in turn altered.

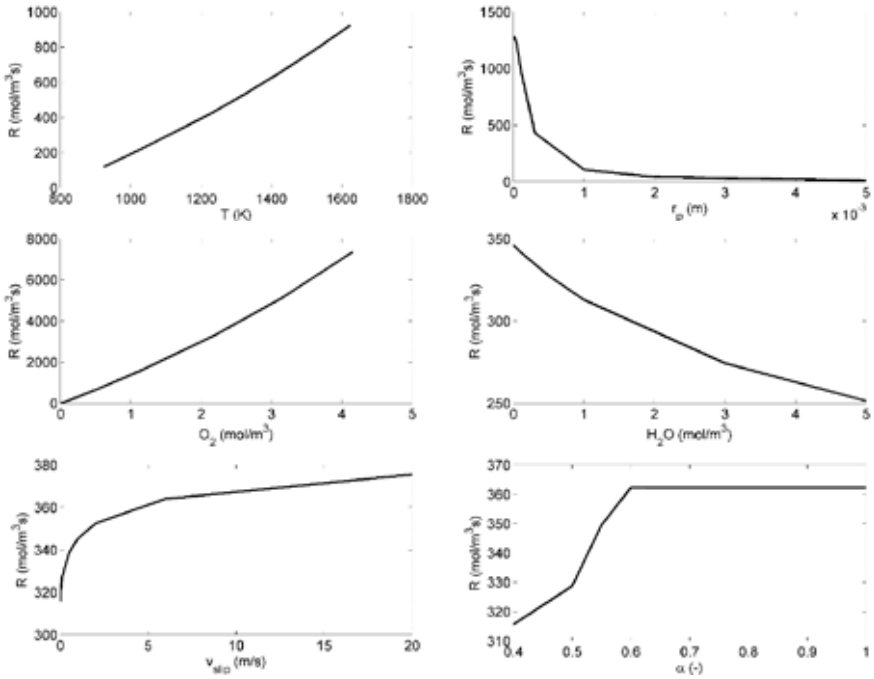

Fig. 2. Effects of temperature, O_2 and H_2O concentration, particle radius, slip velocity and voidage on fuel oxidation rate. The rates are presented relative to the volume of the particle.

Fuel particle size, gas composition and temperature have strong effects on the conversion rate. The effect of H_2O on the combustion rate comes from the fact that gasification reactions produce CO which consumes oxygen and reduces the amount of oxygen available for combustion of char carbon. Although slip velocity and voidage have effects, these effects are minor compared to the main parametric effects. Slip velocity was set in the single particle model at 5 m/s which is in the typical range valid for fuel particles. Since most of char conversion takes place in the dense bottom region, in the present demonstration of the modeling method, the model was written for dense conditions assuming a constant voidage of 0.4. The other considered parameters, bed particle diameter and density had minor effects compared to the concentrations and temperature and they were omitted from the model as input parameters. Thus the model inputs chosen for modeling of char oxidation rate were temperature, O_2, CO_2 and H_2O concentrations and particle size.

Figure 3 shows parametric effects on H_2O and CO_2 gasification rates. Effects of voidage, slip velocity and bed particle properties were again minor and they are omitted from the figure. The effects of temperature and particle size are again significant. Similarly, concentrations of O_2, CO_2 and H_2O affect both gasification rates. The effect of O_2 concentration on H_2O gasification rate is due to increased particle temperature at higher O_2 values. As O_2 concentration increases, CO_2 gasification rate grows both due to increased temperature and due to increased CO_2 concentration inside the particle. Thus we can conclude that the same set of inputs that was selected for modeling of char oxidation rate can be used also as the set of inputs determining the gasification rates.

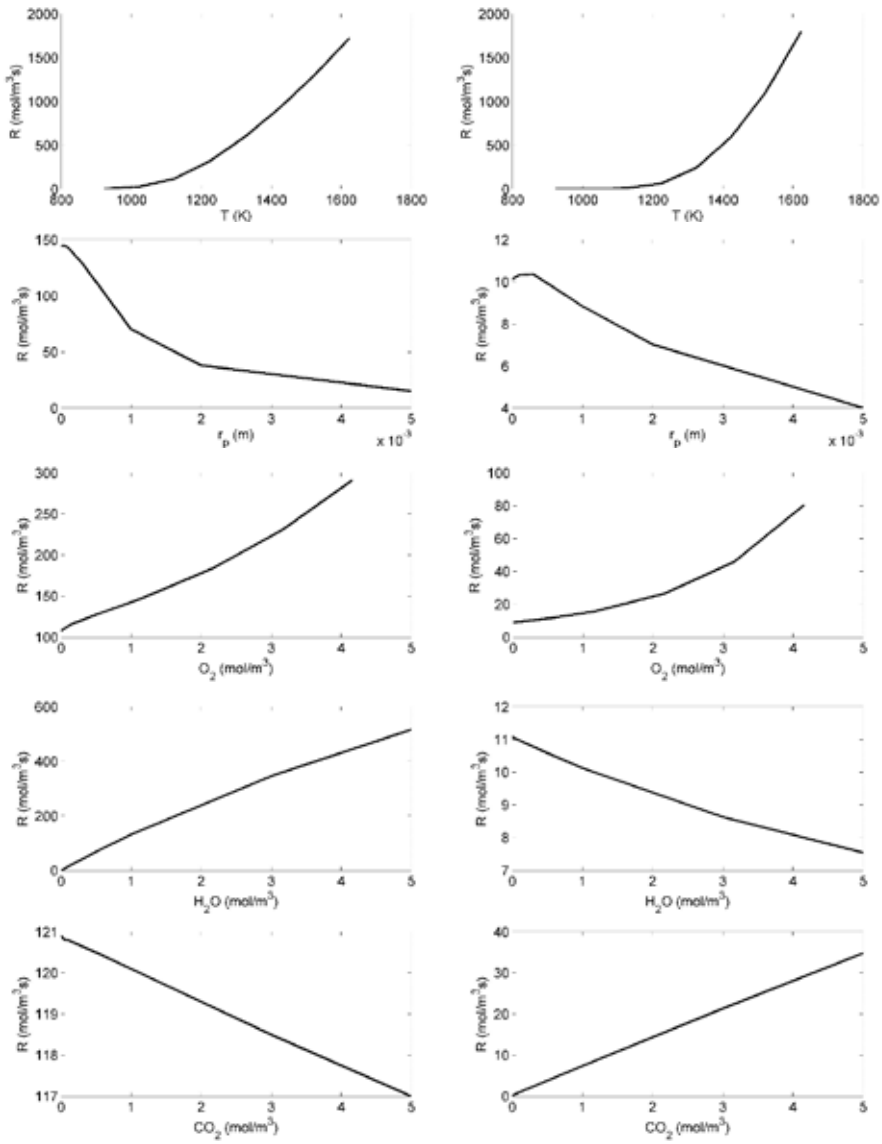

Fig. 3. Effects of temperature, O_2, CO_2 and H_2O concentration and particle radius on H_2O (left) and CO_2 (right) gasification rates.

After the input parameters were chosen, a large data set containing 4000 data points was created by varying the values of the inputs randomly in a wide range of condition. The ranges inside which the variables were varied are shown in Table 1. The data set contains combinations of parameter values that are not realistic in atmospheric combustion conditions but for modeling purpose it was considered safer to extend the range beyond typical values. If a model is needed for pressurized conditions, the ranges should be further widened. The single particle model was used to compute the rates for oxidation and gasification reactions in the 4000 points and the computed net reaction rates and the average particle temperature were collected.

Table 1. The ranges for the input variables in the training set.

	O_2 (mol/m^3)	T (K)	r_p (μm)	CO_2 (mol/m^3)	H_2O (mol/m^3)
MAX	4	1600	4000	11	12
MIN	0	720	10	0	0

NEURAL NETWORK MODELING

In CFD simulation only the net reaction rates are required and not the conditions inside the fuel particle as such. Thus it suffices to express the net reaction rates as functions of the particle size, the temperature and gas composition in the surroundings. As seen in Figures 2 and 3, some of the relations between the variables are highly nonlinear and, moreover, strong cross-effects of changes in particle size, temperature and gas composition are common. Thus a versatile tool for nonlinear empirical modeling is to be preferred to avoid tedious manual work that can be required to find the optimal functional shape and parameter values. Feed forward neural networks serve as a good tool for this type of modelling and hence this approach was followed. The model structure for a NN with a single hidden layer is as follows (Hornik et al., 1989):

$$Y = b_0 + \sum_{i=1}^{N_\sigma} b_i \, \sigma(z_i) \tag{5}$$

$$z_i = a_0 + \sum_{j=1}^{N_{in}} a_{ij} \, x_j \tag{6}$$

where a_{ij} and b_i denote model parameters and x_j the N_{in} input variables. The logistic sigmoid function that produces values between 0 and 1 is given by

$$\sigma(z_i) = \frac{1}{1 + e^{-z_i}} \tag{7}$$

The suitability of the parameters that were selected as model inputs by analysis of the parametric effects were now reconsidered. In the CFD simulation, fuel particles are tracked and their temperature is constantly calculated using an energy balance. Particles that move from hot furnace center to the cooler wall region don't immediately cool down to the temperature that would correspond to the steady state temperature for the particle in the cool surroundings. However, reaction rates inside the particle are dependent on the actual instantaneous particle temperature and thus instead of the temperature of the surrounding gas, the particle temperature, that was also recorded from the single particle modeling, was chosen as one of the inputs. A scaling of the inputs was also done to get the inputs to the same order of magnitude to help in the numerical evaluation of model parameters. The temperature was divided by 1000 and the concentration of O_2 and the particle radius were expressed as logarithms.

The data collected from single particle simulations was used to train the neural network models using the Levenberg-Marquardt (Marquardt, 1963) method. Although it would be possible to include several outputs in a single NN model, it was decided to develop three separate models for the three conversion rates since the nonlinearities and effects of the different inputs were often of different character. It is also a common practice to divide the data into training, test and validation sets. The training set is used to determine the model parameters while the prediction error for the test set is used as an indicator for preventing over-parametrized models and the validation set to confirm the validity of the final model. Instead of using a test set we chose to prevent over-parametrization by analyzing the smoothness of the predictions and the quality of the neurons (models with saturated or dead neurons were rejected). Several model configurations with different number of nodes in the single hidden layer were tested and finally for oxidation and gasification rates, suitable NN models were selected for implementation in a CFD model for CFB combustion. All the three models had seven neurons in the hidden layer (N_σ=7). It is possible that the number of neurons or at least parameters could still be reduced by a pruning procedure where the effect of each parameter is evaluated and parameters with small effects are omitted. This was not done in the present work. The developed correlations are fast to compute and easy to implement in a CFD code.

The correlation between the single particle model predictions and the NN model predictions were excellent, as seen in Fig. 4. The figure shows that at high conversion rates the predictions are slightly less accurate. Analysis of these points showed that they correspond to extreme combustion conditions with high temperatures and oxygen concentrations. Although it would be possible to develop a model that fits also this data better, it was not considered necessary taking into account the low likelihood of encountering these conditions in the furnace.

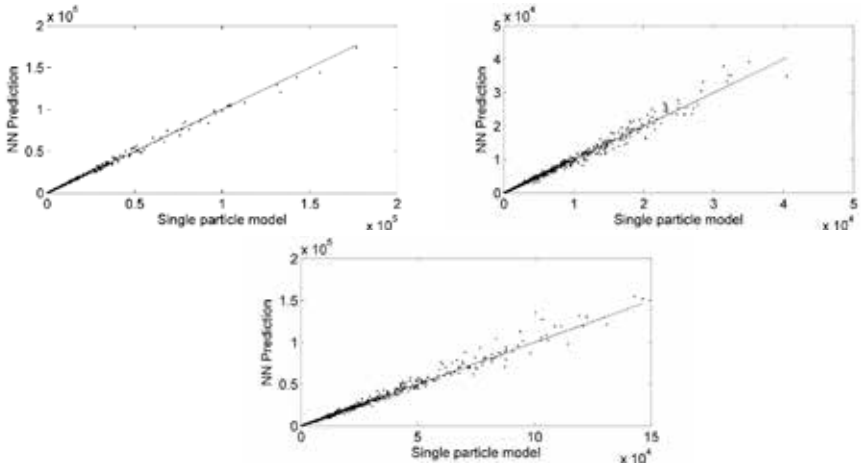

Figure 4. Comparison between single particle model and NN model predictions for the training set data. Top left: oxidation model, top right: CO_2 gasification, below: H2O gasification.

MODEL VALIDATION

To test how well the models function in realistic combustion conditions, a validation data set was created by picking data on gas atmosphere and temperatures from a CFB simulation of a CFB boiler. The range for the conditions is given in Table 2 and the amount of validation points was 7000. Conversion of particles of different sizes in all these conditions was computed with the single particle model and for comparison, reaction rates in the same cases were calculated with the NN models. Figure 5 shows the comparison between single particle model and NN model predictions. In general, the match between NN predictions and the values produced by the single particle model is excellent. There are a small number of data points in which the NN model predicts clearly too low CO_2 gasification rate. The fraction of these points is very small and thus the discrepancy is not expected to lead to noticeable effects in CFD simulations. Although the model could be improved by addition of one or several neurons in the neural net, it was not considered necessary.

Table 2. The ranges for the input variables in the validation set.

	O_2 (mol/m^3)	T (K)	r_p (µm)	CO_2 (mol/m^3)	H_2O (mol/m^3)
MAX	2.59	1110	4000	1.9	2.18
MIN	0.037	908	30	0.035	0.0026

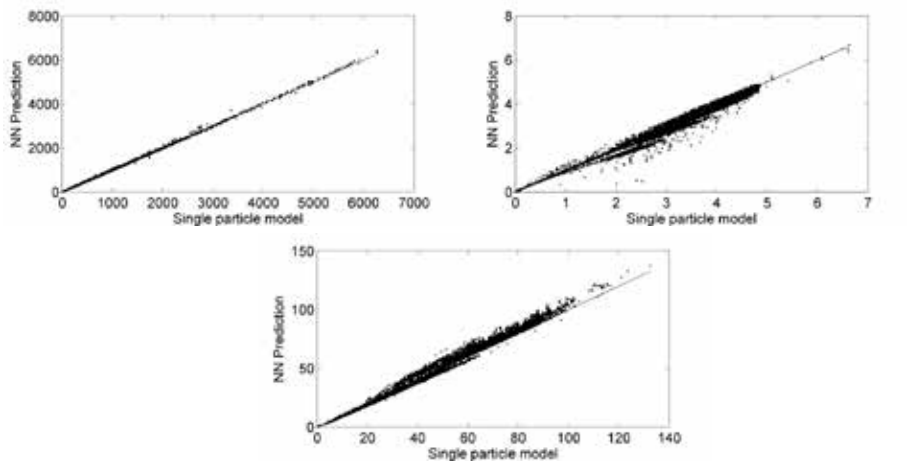

Figure 5. Comparison between single particle model and NN model predictions for the validation set data. Top left: oxidation model, top right: CO_2 gasification, below: H_2O gasification.

DISCUSSION

Conversion rates of different fuels differ and the model parameters should be revised when used for different fuels. It is not practical to directly determine the NN parameters from measurements of the conversion rates since a large amount of data from different conditions would be required. Instead, the reaction rate parameters used in the single particle model could be adjusted to fit a small amount of measurement data after which the single particle model could be used to produce a new training data set for NN parameter estimation. It is unlikely that the character of the dependencies between input variables and the reaction rates would change. Thus the same NN structure can be used and only the parameters need to be determined for each different fuel.

In this paper, only the oxidation and gasification of char was considered. The same modeling procedure has been also used for modeling of NO and N2O chemistry and the models have been implemented in a CFD code.

CONCLUSIONS

In CFD simulation, computation of the conversion of a single particle should be fast. The objective of the present study was to convert a detailed shrinking particle model for coal combustion into a correlation based description that can easily be implemented in a CFD code. The shrinking particle model used as the basis in the work was the one of Konttinen et al. (2002), augmented with expression for gasification rates. In the study, the single particle model was used to produce net reaction rates averaged over particle volume in a wide range of fluidization, temperature and composition conditions. Net reaction rates for combustion and gasification by CO_2 and H_2O and the average particle temperature were produced with the single particle model and from the collected data, the main parameters that determine the conversion rates were identified and a data set with the input variables and the obtained conversion rates was collected.

The data obtained from single particle simulations was used to train neural network models for the reaction rates. Several model configurations with different number of nodes in the single hidden layer were tested and finally suitable NN models with seven neurons in the hidden layer were selected for implementation in a CFD model for CFB combustion. The developed correlations are fast to compute and easy to implement in a CFD code. From the study it can be concluded that the complicated physics and chemistry taking place inside a single fuel particle can be easily expressed in the form of a correlation that is suitable for CFD modeling.

The single particle model used in this study was for bituminous coal. For other fuels, the procedure should be repeated by first fitting the reaction rate parameters of the single particle model to measurement data available for the other fuels and then using the single particle model to create training data for the NN correlation model.

NOTATION

c_i	gas concentration of species i, mol/m^3	T	temperature, K
$D_{e,i}$	effective pore diffusion coefficient, m^2/s	v_{slip}	slip velocity, m/s
ΔH	reaction enthalpy, kJ/mol		
k_g	external mass transfer coefficient, m/s	Greek symbols	
R	reaction rate, mol/s or mol/m^{3}s	α	voidage, -
r	radial position, m	α_{tot}	net heat transfer coefficient, W/(m^2 K)
r_p	fuel particle radius, m	λ_e	effective thermal conductivity, W/(m

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