Grate Furnace Combustion: A Submodel for the Solid Fuel Layer

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Abstract. The reduction of NO_x -formation in biomass fired grate furnaces requires the development of numerical models. To represent the variety in scales and physical processes playing a role in the conversion, newly developed submodels are required. Here, a submodel for the reverse combustion process in the solid fuel layer on the grate is described. The submodel is shown to give good predictions for the velocity of the combustion front as well as for the spatial profiles of porosity, oxygen mass fraction and temperature. These predictions are essential input for NO_x -calculations.

Keywords: Grate furnace, reverse combustion, biomass.

1 Introduction

A popular way of medium small-scale thermal biomass conversion is the use of grate furnace combustion [1]. The operating conditions and design of such a furnace have to be chosen carefully to meet the NO_x emission limits. Numerical models can support the making of these choices, provided that accurate submodels for the phenomena occurring in the oven are available.

The formation of NO_x in the furnace (cf. [1]) is strongly determined by the combustion process in the furnace. Generally, the conversion processes takes place in two zones. In the primary conversion zone, the solid fuel is gasified on a moving grate. In the secondary conversion zone, additional air is supplied to burn out the resulting gas mixture. Due to the low combustion temperatures in both zones, the main source for the NO is the fuel-N (fuel-bound nitrogen). In the solid fuel layer, the fuel-N is released as so-called N-precursors, mainly NH_3 . In the secondary conversion zone, part of these precursors is converted to NO .

The combustion process as well as the NO_x -formation process is highly complex due to the different physical phenomena involved, i.e. transport of heat and mass as well as chemical reactions. Furthermore, a wide range of length scales is involved. The overall combustion process is determined by the conversion of single particles, occurring at a typical length scale of a particle diameter. Multiple particles are converted simultaneously in a reaction wave, propagating

trough the solid fuel layer in the primary conversion zone on a length scale of the bed height. Finally, the gases originating from the solid fuel layer burn out and transfer their heat to the boiler present in the oven at a length scale given by the dimension of the oven.

To represent the variety in scales and physical processes affecting the NO_x -formation process, submodels for (i) the combustion process in the solid fuel layer, (ii) the release of N-precursors from the solid fuel layer (iii) the gas phase combustion process and (iv) the oxidation of the N-precursors are required [2]. Without a submodel for the combustion process in the solid fuel layer, advanced models for the secondary combustion zone (cf. [3]) have to operate with a boundary condition based on measurements just above the solid fuel layer, which strongly restricts their flexibility (cf. [4]).

In developing a model for the solid fuel layer, its resemblance to a fixed bed combustion process can be exploited. In a reference frame traveling at the same velocity as the grate, the combustion process is similar to reverse combustion in a fixed bed [5]. In this mode, air is flowing in the upward direction through the fuel layer, while the reaction front propagates downward. Reverse fixed bed combustion processes can be described with 1-dimensional models.

Existing 1-dimensional numerical models for reverse fixed bed combustion (e.g. [6], [7]) and coal have the disadvantage that due to the great amount of detail in the equations and their time-dependent formulation, they require calculation times that are too long to study changes in furnace design and operating conditions [4]. The complexity may also lead to numerical difficulties (cf. [8]). Application of sensitivity analyses to these models is generally not reported, which raises the question up to which extent their complexity and the resulting calculation times are justified.

The present work addresses the need for a model that is able to describe the reaction front propagating in the solid fuel layer with only the essential processes and at low computational costs. Therefore, a limited set of equations based on a model from the literature [9] is used. The predictions of the model are at the length scale of the bed, while in the model chemistry and transport processes at the level of a single particle are accounted for. At the moment the model presented here is operating with a parameter set for coal combustion, but as the combustion process for wood-like biomass is essentially the same, the model can be adapted for this.

In this work, two important new aspects of the model are presented. Firstly, it is shown that this model can be solved also numerically, while in the past it has been solved analytically only [10]. This opens the possibility to extend the model for increased accuracy and flexibility if necessary. Secondly, it is shown that stationary solutions for the reverse combustion process can be obtained by using a reference frame attached to the combustion front. This enables convenient performance of parametric studies and results in fast calculation times. In addition, with the numerical analysis it can also be shown that the effect of heat and mass and heat transfer limitations in the fuel bed lead to a change

in flame structure and thus to the applicability of analytical solution methods. This study is presented elsewhere (cf. [11]).

An important feature of the model is that it can be combined with a submodel for the release rates of N-precursors. These release rates are strongly determined by the conversion rate and temperature, (cf. [12]), two quantities that can be predicted with the model. These quantities can serve as input for a submodel consisting of N-precursor release rates based on measurements in a heated grid reactor (cf. [13]) or TGA (cf. [12]).

It is the purpose of this paper to illustrate the advantages of the numerical implementation of the model and the possibilities it offers to serve as a submodel for grate furnace combustion. An extensive comparison of model results with experiments falls not within the present scope. Suffice it to remark that the model currently predicts conversion rates that have the correct order of magnitude compared to experimental results (eg. [14]) which is good, considering that i) the model is not highly detailed, while fixed bed conversion is a complex process, ii) no adaption of the model constants was performed to fit the model to the measurements, iii) there are large uncertainties in some of the model constants and iv) there are large uncertainties in experimental results reported (compare [10] with [14])

The outline of this paper is as follows. First, the model equations are discussed (Sec. 2). Then, it is shown that the model can predict spatial profiles of the variables and the conversion rate of the solid material (Sec. 3). Finally, the conclusions are presented (Sec. 4).

2 Model Equations and Data

In this section a short review of the model equations and data presented in Ref. [10] is given. The model consists of a set of three equations for the porosity of the fuel bed ϵ , the temperature T and the oxygen mass fraction Y as a function of the spatial coordinate x . In order to obtain this set, the original time-dependent model equations have been transformed to a reference frame traveling at the same velocity as the combustion front [9]. This results in:

$$v_s \frac{d}{dx} (\rho_s (1 - \epsilon)) = -R \quad (1)$$

$$v_s \frac{d}{dx} (\epsilon \rho_g Y) + \frac{d}{dx} (\epsilon \rho_g v_g Y) - \frac{d}{dx} \left(\rho_g D \frac{dY}{dx} \right) = \nu R \quad (2)$$

$$v_s \frac{d}{dx} ((1 - \epsilon) \rho_s c_{ps} T + \epsilon \rho_g c_{pg} T) + \frac{d}{dx} (\epsilon \rho_g v_g c_{pg} T) - \frac{d}{dx} \left(\Lambda \frac{dT}{dx} \right) = -\Delta H_r R \quad (3)$$

Here, v_s is the velocity of the solid, which is moving due to the change in reference frame. The first terms on the rhs. of each equation are convective fluxes involving v_s . These result from the transformation of time-derivatives in the original reference frame. Other symbols in this set of equations are the reaction

source term R , reaction enthalpy ΔH_r , effective coefficients for dispersion D and conduction Λ as well as specific heat c_p and density ρ for gas and solid (subscripts g and s , respectively). The boundary conditions are given at the unburnt side (u ; $x \rightarrow -\infty$) and burnt side (b ; $x \rightarrow \infty$)

$$\epsilon|_u = 0, \quad Y|_u = Y_u, \quad T|_u = T_u; \quad \left. \frac{dY}{dx} \right|_b = 0 \quad \left. \frac{dT}{dx} \right|_b = 0. \quad (4)$$

In this paper, instead of using v_s and v_g , results are presented in terms of the gas mass flux and solid mass flux at the unburnt side, given by

$$m_{gu} = \epsilon_u \rho_{gu} v_{gu}; \quad m_{su} = (1 - \epsilon_u) \rho_s v_{su}. \quad (5)$$

Summarizing, the stationary model equations (1,2) and (3) together with the boundary conditions can be used to obtain $\epsilon(x)$, $Y(x)$ and $T(x)$ as well as m_{su} as a function of gas mass flux m_{gu} .

Expressions for the reaction source term, the diffusion coefficient and the conductivity coefficient are required to solve the model. To obtain an expression for R the heterogeneous surface reaction of coal with oxygen

is used. As measurements indicate that the primary product in the reaction zone is CO_2 [10], this is a reasonable assumption. The volumetric reaction rate per unit volume can be expressed by

$$R = \frac{1}{k_r^{-1} + k_m^{-1}} S^{2/3} \rho_g Y. \quad (7)$$

Here, k_r is an Arrhenius rate constant, k_m a mass transfer coefficient and S the specific surface area of the fuel bed. Introducing the dimensionless mass transfer coefficient,

$$K_m = \frac{k_m}{k_r} \quad (8)$$

it can be seen that for $K_m \rightarrow \infty$, R is limited by kinetics, while $K_m \rightarrow 0$ indicates that R is limited by mass transfer effects. In the kinetically limited case, the expression reduces to that given by Field [15]:

$$R = k_r \rho_g Y S. \quad (9)$$

with k_r given by

$$k_r = A_f T \exp\left(-\frac{E_a}{RT}\right), \quad (10)$$

in which the pre-exponential factor is indicated with A_f and the activation energy by E_a . The specific surface area in the rate expression can be related to particle properties. For spherical particles of diameter d_p in an SC (simple cubic)

structure reacting as a shrinking core, the specific surface area during conversion can then be expressed by [10]

$$S = S_u \left(\frac{1 - \epsilon}{1 - \epsilon_u} \right)^{2/3}. \quad (11)$$

Finally, expressions for the gas density, the effective conductivity the dispersion coefficient and the mass transfer coefficient are needed. The gas density is given by

$$\rho_g = \rho_{gu} \frac{T_u}{T_b}. \quad (12)$$

Correlations for Λ , D and k_m are given in [10]. The model equations and additional data are implemented in the one dimensional laminar flame code Chem1d [16].

Table 1. Data used for the calculations for a propagating reaction front in a bed of coal particles [10]

Parameter	Unit	Value
T_u	K	288
ΔH	J g ⁻¹	28.9×10^3
c_{ps}	J kg ⁻¹ K ⁻¹	1.8
ρ_s	g cm ⁻³	1220×10^{-3}
ρ_{sa}	g cm ⁻³	470×10^{-3}
d_p	cm	2.5
$\rho_{gu}(T_u)$	g cm ⁻³	1.226×10^{-3}
c_{pg}	J kg ⁻¹ K ⁻¹	1.13
Y_u	—	0.23
A_f	cm K ⁻¹ s ⁻¹	6×10^4
E_a	kJ mol ⁻¹	150
ν	—	2.67

3 Results

Model results consist of spatial profiles of ϵ , T and the heat release $\dot{q}$. Here, we present solutions for varying m_{gu} (cf. Fig. 1). The latter quantity can be determined by the equation $\dot{q} = -\Delta H_r R$ and is a measure for the magnitude reaction source term. The results show that with increasing m_{gu} , $\dot{q}$ increases. At the same time, the width of the boundary layers in the profiles for T and Y increases. Due to the increased flow of air, the conversion of the solid fuel ϵ_b as well as T_b become higher.

From the spatial flame profiles for different m_{gu} , the conversion ϵ_b as well as T_b can be determined as a function of m_{gu} (cf. Figs. 2b, 2c). By using T_b in the evaluation of K_m (cf. (8)), K_{mb} can be determined (cf. Fig. 2d). Furthermore, m_{su} results from the calculations (cf. Fig. 2a). It can be observed that m_{su} initially increases when m_{gu} increases, until a maximum is reached. Then, m_{su}

Fig. 1. Spatial flame profiles for varying gas mass flux. Results for Y and ϵ (a) and T and $\dot{q}$ (b). The arrows indicate results obtained with increasing m_{gu} from $m_{gu} = 4.9 \times 10^{-3} \text{ g cm}^{-2}\text{s}^{-1}$ to $m_{gu} = 14.6 \times 10^{-3} \text{ g cm}^{-2}\text{s}^{-1}$ in steps of $2.4 \times 10^{-3} \text{ g cm}^{-2}\text{s}^{-1}$.

Fig. 2. Flame parameters as a function of gas mass flux for varying activation energy. Results for the solid mass flux (a), the porosity (b), the temperature (c) and dimensionless mass transfer coefficient (d). Solid line: $E_a = 150 \text{ kJ mol}^{-1}$, dashed line: $E_a = 160 \text{ kJ mol}^{-1}$, dotted line: $E_a = 170 \text{ kJ mol}^{-1}$.

decreases until extinction takes place. The shape of the curve of m_{su} as a function of m_{gu} (Fig. 2) was explained in earlier works in terms of the counterbalancing effects of the increased oxygen supply to and and increased convective heat transport out of the reaction zone with increasing m_{gu} (cf. [17]). The temperature T_b and porosity ϵ_b increase continuously with increasing m_{gu} . (Due to limitations

of the current numerical implementation, the extinction point $\epsilon_b = 1$ is not reached completely). The dimensionless mass transfer coefficient K_{mb} (i.e. K_m evaluated at T_b) shows that for low m_{gu} , the source term is controlled by kinetics ($K_{mb} > 1$). At $m_{gu} \sim 1.0 \times 10^{-3} \text{ g cm}^{-2} \text{ s}^{-1}$ mass transfer effects begin to play a role ($K_{mb} < 1$). Furthermore, it can be seen that all parameters are sensitive to changes in E_a .

A typical calculation time to obtain results for a variation of m_{gu} from zero up to the extinction point is only ten minutes on a PC. Furthermore, with other models for coal beds with an instationary formulation (e.g. [18]), it is no longer necessary to wait until a steady state is reached when a parameter is varied.

4 Conclusions

From the numerical results presented in this paper, it can be concluded that the two most important quantities that determine the release of the N-precursors can be predicted, namely the front velocity and temperature. These quantities can be determined as a function of gas mass flow, the main controlling parameter in a grate furnace. In the calculations, both kinetics and mass transfer limitations can be taken into account. Furthermore, the effect of fuel parameters (particle size and bed density) that show strong variations in practical combustion processes has been included via the correlations used to determine the model coefficients.

The implementation of a stationary set of equations as is performed here has two important advantages. Firstly, the calculation times are short. This makes the method proposed here suitable for application as a submodel in a grate furnace. Moreover, the model can be extended further with additional important phenomena and still remain within the limits of reasonable calculation times. In addition, the instationary implementation makes it convenient to perform parametric studies. This makes it achievable to study the effect of additional phenomena included in the model by means of a sensitivity analysis to determine their effect on the velocity of the reaction front, the temperature and the structure of the reaction zone.

First, the model will be extended to describe the additional chemistry necessary for biomass conversion by using the Chem1D modules for the gas phase kinetics. It is also planned to include the effect of other parameters that are shown to have a large impact on the combustion process in practical applications, e.g. the moisture content of the fuel.

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