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Numerical Modelling of Grate Combustion

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Ústav procesního a ekologického inženýrství

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Numerické modelování spalování na roštu

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CONTENTS

1 INTRODUCTION

During the past twenty years, grate-fired systems have received significant attention by researchers involved in combustion science. It is not only because renewable and environmentally friendly energy sources such as biomass have been found as a promising alternative to fossil fuels. Also incineration in grate-type furnaces has become a widely-used method of municipal solid waste disposal.

Many experimental measurements have been carried out in order to improve the effectiveness of energy utilization as well as to reduce the pollutant emissions and undesirable effects of combustion products on heat transfer surfaces. However, due to the difficulty and increasing costs of experiments, the research has also been focused on development of a reliable computational model as a supporting tool for design and optimization of combustion systems.

1.1 MOTIVATION

Current Computational Fluid Dynamics (CFD) codes such as ANSYS FLUENT [3] have become very practical tools for analysis of all kinds of solid fuels utilization systems. However, quality of simulation results is strongly affected by the quality of input data [26]. Therefore, in order to develop a reliable CFD model, care must be taken when preparing the mesh and defining not only physical and chemical models, but also boundary conditions and additional models (e.g. a model of deposit formation on surfaces of heat exchangers, see [11, 12]), which are sometimes necessary to incorporate into the CFD code to adjust the solution procedure and enhance capabilities of the CFD modelling tool [1, 26].

This work concerns CFD modelling of grate combustion as widely used technology in biomass and municipal solid waste combustion for heat and power production [25]. A typical 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. 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 must be supplied as inlet boundary conditions. The situation is schematically shown in Figure 1. Specification of the type and values of boundary conditions is crucial in any numerical problem. Especially, in case of grate combustion modelling, where there is a strong coupling between processes occuring inside the fuel layer and in the over-bed region, inappropriate treatment of the boundary conditions may lead to inaccurate results of a simulation, mainly in the vicinity of the fuel bed [26]. Apparently, the degree of approximation of in-bed processes is important.

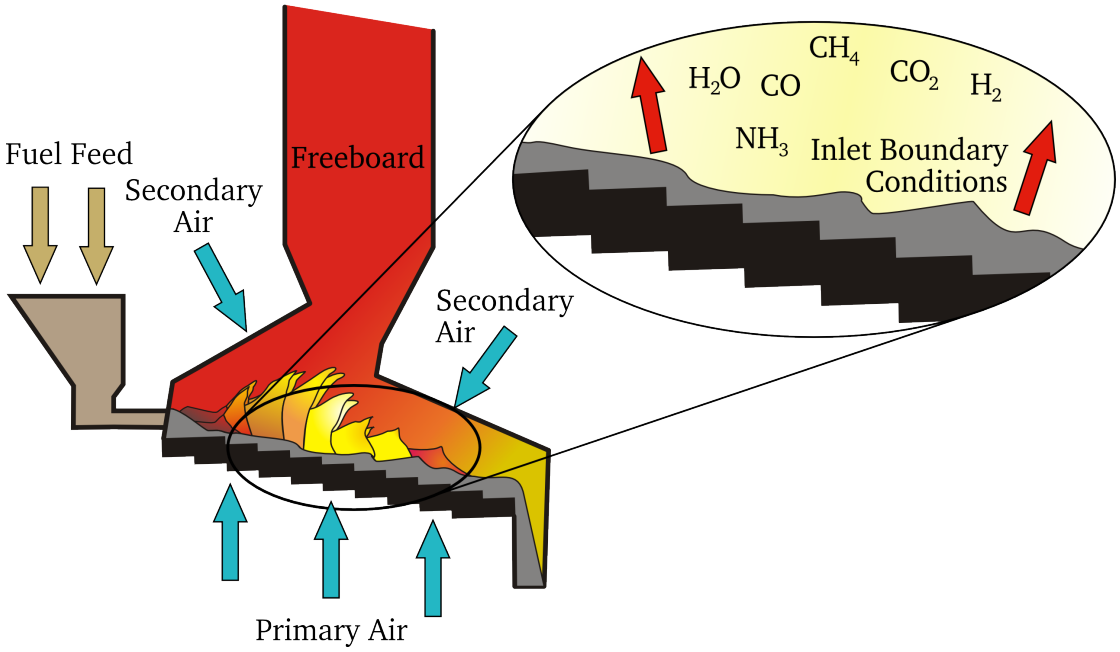

Figure 1: A scheme of a grate incinerator with boundary conditions at the grate.

A promising method for estimating heat and mass fluxes at the grate is based on a coupled-modelling approach, in which a fuel bed is physically separated from the rest of the furnace (so-called freeboard) and processes, that take place within the bed during combustion, are solved by using a standalone numerical bed model. These two models are coupled by boundary conditions at the common interface. While the freeboard model passes to the bed model an incident radiation heat flux, which initiates combustion in the bed, the bed model returns to the freeboard model properties of flue gas leaving the bed as results of in-bed simulation. This procedure is iteratively repeated until the radiation heat flux does not significantly change providing for coupling of in-bed and freeboard processes. This concept has been used in a few studies on grate combustion of solid fuels, e.g. [16, 22, 28].

However, as it is stressed in [27], 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, see e.g. [2]. 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. This may lead to inaccurate results of freeboard combustion predictions as the accuracy depends, among others, on the quality of input data [26].

1.2 OBJECTIVES AND SCOPE OF THE THESIS

This work is focused on numerical modelling of grate combustion. The first objective is to develop and implement a stand-alone conservative numerical model of packed-bed combustion such that it may serve as a tool for both study and analysis of various processes in the bed and calculation of boundary values in the coupled-model methodology. The emphasis is put on the conservativeness property of the model. Therefore, a method for control of mass and energy balance over the system is developed, by means of which the model can be checked and corrected for various errors to yield a conservative model. The method is also applied to several of simulations to determine a suitable value of convergence criteria in order to produce acceptably low mass and energy imbalance. Such a parametric study has, to the author's knowledge, not been performed yet and therefore the result contributes to better understanding of numerical modelling of grate combustion, especially in the setup of a numerical model and parameters of solver for the control of the convergence. Other physics-related issues including propagation of drying and char oxidation reaction fronts are addressed and investigated by means of numerical simulation using the computer code developed within this work.

The second objective is to develop a library of user-defined functions for the commercial CFD software ANSYS FLUENT for coupling the bed model with a freeboard model of a real combustion unit in order to specify the boundary conditions indirectly using results from in-bed simulations. The library of functions should be general enough to be easily applied for a wide range of grate furnace models.

2 BED MODEL SETUP AND IMPLEMENTATION

This chapter introduces a mathematical model of packed-bed combustion, which has been developed within this work. The description starts with a choice of a suitable kind of the model. Also the most important parameters of the model are described and discussed. A part of the chapter is devoted to numerical methods used for solving discretization and solution of governing equations. The implementation of the model and numerical methods into a computer program GRATECAL 1.3 is described briefly in the last section.

2.1 BED MODEL TYPE

The firts step in development of a model is the choice of a suitable level of approximation with respect to purposes and needs of modelling. Selection of the kind of the model and included physical models is made on the following requirements:

- **Coupled simulation.** The stand-alone bed model should be suitable for coupled simulation of grate combustion, preferably in (but not limited to) units with continuous feeding. The model is expected to improve quality of input data for a freeboard CFD model of a grate combustor. In most part, this is concerned with calculation of mass and heat fluxes entering the freeboard, which otherwise would be only rougly estimated in the absence of the bed model.

- **Level of approximation.** The bed model should allow to analyse main combustion parameters including various process rates, heat transfer rates, temperatures, mass fluxes, concentrations of flue gas species and amount of mass of constituents remaining in the fuel. On the other hand, too much detailed and complex model could be computationally very demanding leading to considerably longer computational times, which is typical for particle-resolved macroscale models.

- **Conservativeness.** In order to achieve improved quality of input data, the bed model must be conservative, i.e. the gas must carry a correct amount of mass and energy. This is an essential requirement as any kind of model must obey basic principles of physics such as conservation laws.

According to foregoing requirements, it is necessary to treat gas and solid as two separate, though coupled, phases and represent their physical properties by specific variables. Since fuel beds in industrial grate furnaces occupy large volume with a vast number of particles, it is reasonable to consider the bed a continuous porous layer, as modelling of individual particles would be an enormous task in terms of computational requirements. These featuers are typical for heterogeneous models with continuous solid and gas phases [4], so this class of models is chosen as a suitable level of approximation.

2.2 MATHEMATICAL MODEL SETUP

The one-dimensional transient (1D) model corresponds with an experimental fixed-bed reactor, that belongs to a group of so-called large reactors [5] and can be schematically sketched as in Figure 2. They consist of a thermally insulated cylinder where all processes take place in one direction only. The (possibly preheated) primary air enters the bed through a grate at the bottom of the furnace and flows in plug flow through the fuel layer to the top. The fuel is ignited by a burner or an electric heating device placed above the top of the bed. Such type of a reactor is suitable for batch-type experiments [17, 18, 30]. The model describes unsteady combustion in one spatial coordinate along the bed height. It is important to note that transient solutions of such a system can also be transformed to represent a 2D bed by the so called walking-column

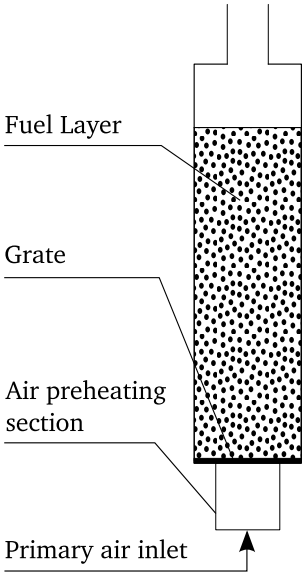

Figure 2: Schematic diagram of an experimental reactor.

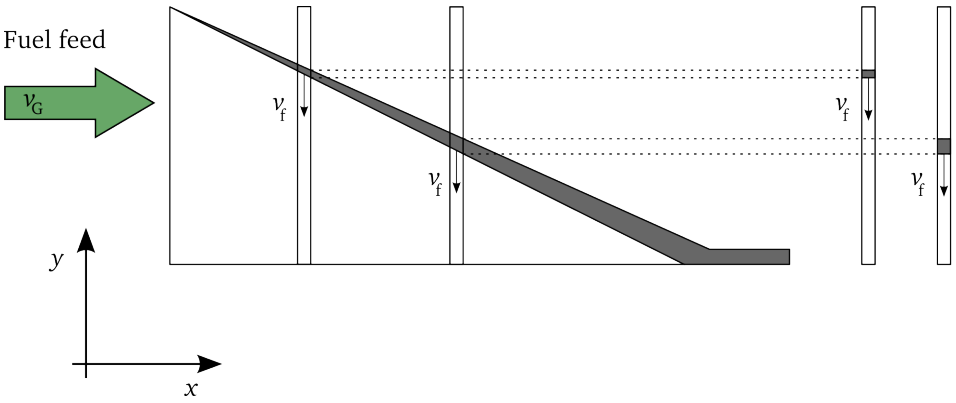

Figure 3: Walking-column approach.

method as shown in Figure 3. The fuel is fed from the left onto the grate and is ignited from the top of the layer. By taking a thin vertical slice of the bed at a position x and following the slice as it is moved on the grate towards the ash pit by known velocity v_G, the reaction front travels down from the top of the column with unknown velocity v_f. In this manner, transient solution of a one-dimensional reactor can be related with a corresponding position on the grate by the simple relation $x = v_G t$, so a continuous operation is represented by a transient one-dimensional batch-type simulation [4].

2.2.1 Model Assumptions

The assumptions made upon the 1D model are adopted mainly from [29]. It is assumed that the fuel bed can be treated as a continuous porous layer consisting of gas and solid phases. Fuel particles are considered thermally thin, i.e. intra-particle temperature gradients are negligible. Fuel consists of four major

species - moisture, volatile matter, char and ash. Combustion can be divided into four sub-processes: moisture evaporation, volatile release/char formation, combustion of volatiles and combustion of char. The gas flow through the porous layer is incompressible, gas is in plug flow and can be described by the ideal gas law. Pressure drop along the bed height is neglected. The gas is a mixture of species $H_2O, O_2, CO_2, CO, H_2, N_2$, light hydrocarbons and tar represented by $CH_4, C_xH_yO_z$, respectively. The radiative heat transfer inside the bed can be modelled by effective thermal conductivity.

2.2.2 Governing Equations and Some Model Parameters

The model is described by a system of partial differential equations of the form [19, 27]

$$\underbrace{\frac{\partial\left(\epsilon\rho\phi\right)}{\partial t}}_{\text{unsteady term}} + \underbrace{\nabla\cdot\left(\epsilon\rho\mathbf{v}\right)}_{\text{convection term}} = \underbrace{\nabla\cdot\left(\Gamma\nabla\phi\right)}_{\text{diffusion term}} + \underbrace{S_\phi}_{\text{source term}}, \tag{1}$$

which is commonly called a general transport equation, where ϵ [-] is porosity of the phase, ρ [kg/m^3] is density, $\mathbf{v}$ [m/s] is a vector of interstitial velocity, ϕ is transported (scalar) quantity, Γ is diffusion coefficient and S_ϕ includes all source terms. The product $\epsilon\rho$ is called bulk density. By giving the variables ϕ, Γ, and S_ϕ physical meanings with appropriate units, Equation (1) becomes a governing equation for heat, mass or momentum transfer. Examples of substitutions for the general coefficients by certain physical quantities commonly encountered in bed models are listed in Table 1.

Equation	ϕ	Γ	S_ϕ
Continuity	1 [-]	0 [kg/m s]	Heterogenous reaction rates r [kg/m^3 s]
Species	Mass fractions of i-th species Y_i [kg/kg]	Product of bulk density and effective mass dispersion coefficient $\epsilon\rho D_i$ [kg/m s]	Rate of production or consumption of species r_i [kg/m^3 s]
Energy	Specific enthalpy h [J/kg]	Effective thermal conductivity divided by specific heat capacity λ/c_p [kg/m s]	Heat transfer rates $\dot{q}$ [W/m^3]

Table 1: Physical meanings of coefficients of the general governing eqation with corresponding physical units for transport equations in the bed model.

Governing equations are based on the reference [29], however, several modifications are introduced regarding definition of source terms, boundary conditions and empirical formulas for calculation of certain physical quantities. Mass and energy transport is modelled by gas and solid continuity equations (solved for mass flux $\epsilon_\mathrm{b}\rho_\mathrm{g}\mathbf{v}_\mathrm{g}$ [kg/m^2 s] and solid density ρ_s, species equations written for gas and solid species mass fractions $Y_{i,g}, Y_{j,\mathrm{s}}$ [kg/kg], respectively, and energy equations solved for gas and solid sensible enthalpies $h_\mathrm{g}, h_\mathrm{s}$ [J/kg], respectively. The original definition of the source term in the gas species equations was incorrect (as described later in 3.3), so it has been reconciled in order to satisfy mass balance of the system. The reconciled source term is $S_{Y_i} = r_i + \epsilon_\mathrm{b}\sum_j r_{i,j}$ [kg/m^3 s], where r_i is rate of production of mass due to drying, pyrolysis and char oxidation, while $\epsilon_\mathrm{b}\sum_j r_{i,j}$ is total rate of mass production/consumption of the specie i due to homogenous reactions.

Following the discussions in one of the author's work [9] and that the approaches of modelling heat and mass transfer were inconsistent with respect to heat and mass transfer analogy [21], a different model of thermal dispersion of the fuel has been adopted from Yang et al. [22].

In addition, two different models of drying have been used and compared in simulations, namely the diffusion-limited rate model (see e.g. [29]) and a modified first-order kinetic rate model, which was applied to modelling of biomass combustion in [14] and is expressed as

$$r_\mathrm{dry} = 2.822\cdot 10^{-4}\exp\left(-\frac{10584}{T_\mathrm{s}}\right)\left(1-\epsilon_\mathrm{b}\right)\rho_\mathrm{s}Y_{\mathrm{H_2O,s}}\left|T_\mathrm{s}-475\right|^7\ [\mathrm{kg/m^3\,s}], \quad (2)$$

where T_s [K] is solid temperature. While char oxidation rate has been adopted from [3, 11], the rate of pyrolysis as well as chemical composition have been taken from [29]. However, chemical formula and lower heating value of tar have been recalculated in order to match mass and energy balance of the fuel.

Boundary conditions at the grate are given by the operating conditions, i.e. primary air enthalpy (or temperature), mass flux and concentrations of species, whereas zero enthalpy gradient is prescribed for solid phase. At the bed top, zero gradients are assumed for gas enthalpy and species mass fractions, while radiation heat flux is prescribed for the solid enthalpy.

2.3 NUMERICAL METHODS

Since governing equations of the bed model are coupled and nonlinear, numerical methods are employed to solve the system of equations. Equation (1) is discretized by the finite volume method. Convective term is approximated by the power law scheme [15], the diffusion term is treated by the second-order central-difference scheme and the implicit Euler method is used for approximation of time integrals. Discretization leads to a set of nominally linear equations

[15]. The convergence of iterations is judged by scaled residuals (nondimensional) as described in [3].

2.3.1 Special Treatment of Process Rates

Beside common techniques such as under-relaxation, linearization of source terms and adaptive time stepping, also an original method of treatment of process rates has been used to ensure that the mass of species is conserved during heterogeneous processes. It is based on a limiting value of the rate according to the initial amount of mass of a certain specie being consumed and expressed as

$$r_{\mathrm{lim}} = \min(r, m^0/(V\Delta t)) \qquad [\mathrm{kg/m^3\,s}], \tag{3}$$

where m^0 [kg] is initial mass of the specie being consumed in the volume V [$\mathrm{m^3}$] during time Δt [s].

2.3.2 Note on Discretization of Effective Dispersion Coefficients

It has been found during testing simulations, that significantly less iterations are needed to obtain a converged solution, when the turbulent term in the dispersion coefficients (see e.g. [21]) is omitted. This behaviour is believed to be caused by an inappropriate interpolation of Γ to the cell faces, which is needed after integration of the diffusion term. The diffusion term is of the form (in 1D case)

$$\frac{\partial}{\partial y}\left(\left(\Gamma_m + \Gamma_t(v)\right)\frac{\partial \phi}{\partial y}\right) = \left(\frac{\partial \Gamma_m}{\partial y} + \frac{\partial \Gamma_t(v)}{\partial y}\right)\frac{\partial \phi}{\partial y} + \left(\Gamma_m + \Gamma_t(v)\right)\frac{\partial^2 \phi}{\partial y^2}, \tag{4}$$

where Γ is split into two parts with a molecular contribution denoted by Γ_m and turbulent contribution $\Gamma_t(v)$, which is a function of velocity v. The turbulent part is now much like the convection term of the general transport equation (1), for which a kind of upwind discretization scheme must be used in order to obtain physically realistic and stable solutions. However, the diffusion term is interpolated by arithmetic or harmonic mean as it is common for diffusion coefficients, so the effect can be similar to central-differencing scheme, if it is applied to the convection term. A remedy could be to interpolate the turbulent part using an upwind technique.

2.4 SIMULATION TOOL WITH GUI

The governing equations together with all physical relations for equation coefficients and numerical methods and techniques mentioned before have been implemented into a computer program, which has been named GRATECAL. It has been developed in the MATLAB environment [13]. The module-based computer program is capable to predict the drying, devolatilization and char oxidation as

Figure 4: Main window of the program GRATECAL.

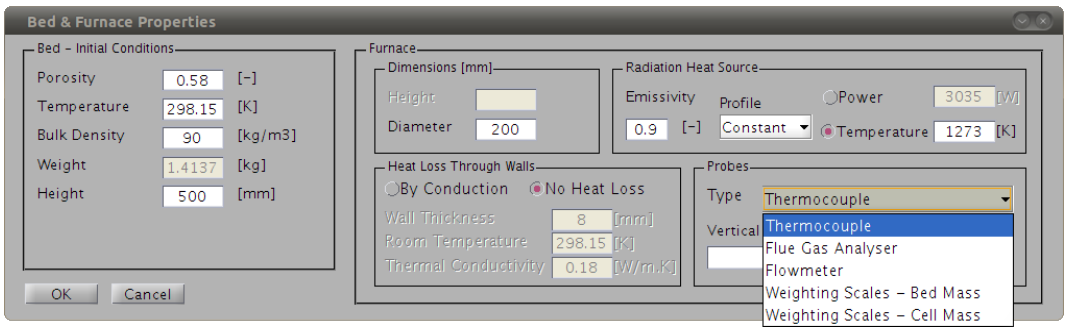

Figure 5: A list of probes available for data recording.

standalone combustion stages as well as to run a full batch-type simulation including all processes together. A graphical user interface (GUI) has also been implemented to make the application user-friendly. The program GRATECAL may serve as a tool for detailed analysis of physical and chemical phenomena, that take place in a packed bed during heat-up, drying, devolatilization and char oxidation. Through graphical tools, temperature, concentrations or flow fields can be viewed along the bed height as well as the propagation of reaction fronts.

As shown in Figure 4 (left), the main window of the computer program consists of a menu bar and a button to start the simulation. Four child windows for specification of simulation parameters are accessible through the `Define` pull-down menu, see Figure 4 (right). These include setting the gas and fuel properties (initial conditions, primary air properties, composition, fuel type, proximate and ultimate analysis of the fuel, etc.), bed and furnace properties (see Figure 5), processes of interest (Figure 6), and solver parameters. By default, scaled residuals of solution variables are plotted after each time step (see Figure 7). Since an experimental reactor is equiped with various measuring probes, the used instrumentation can be selected from the drop-down list of **Bed & furnace properties** child window as it is shown in Figure 5. The selection of probes determines the kind of data that are recorded during the simulation and hence will be plotted after the simulation finishes.

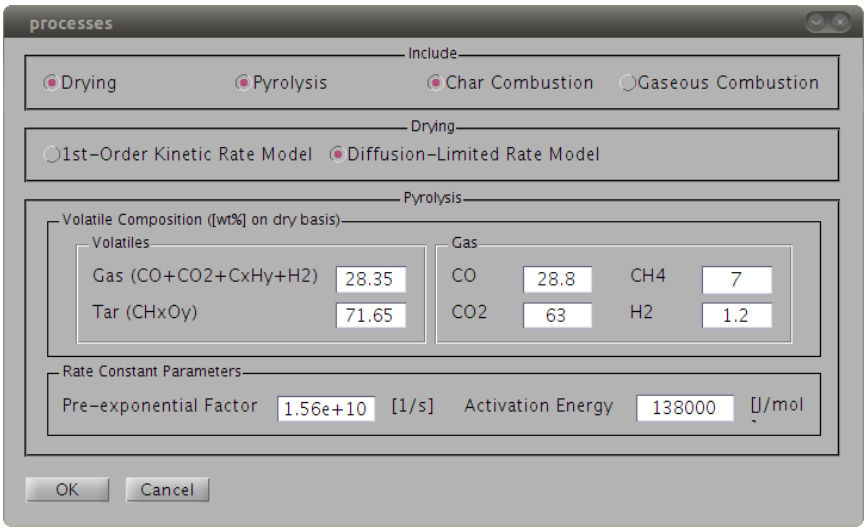

Figure 6: Processes child window for a selection of combustion sub-models.

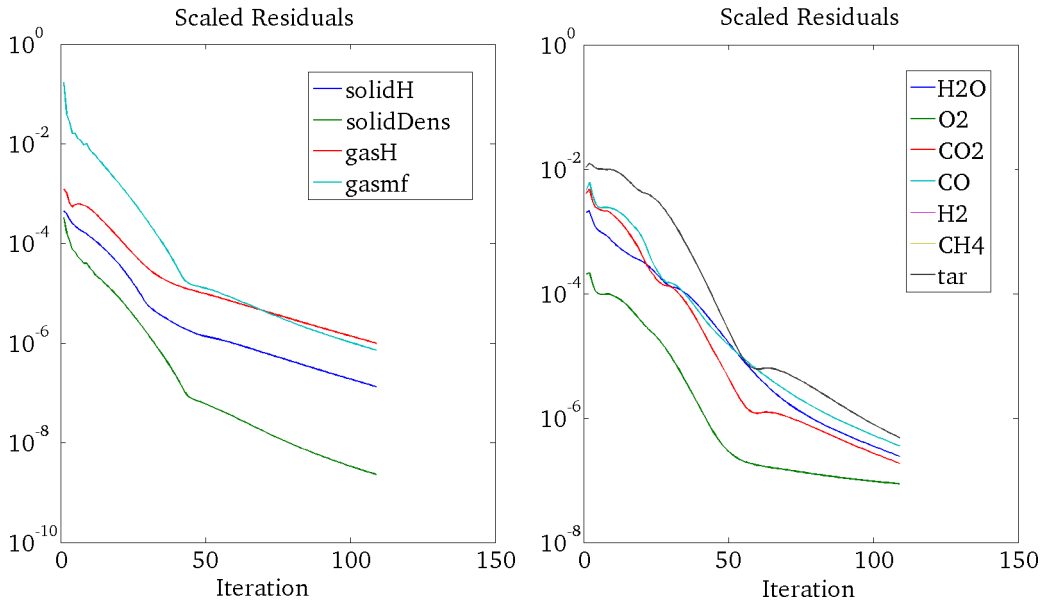

Figure 7: Plots of scaled residuals.

2.5 SUMMARY

A mathematical model of packed-bed combustion have been developed. Development has been based on the existing bed models, however, certain modelling parameters, e.g. mass production source terms have been reconciled in order to yield a conservative numerical bed model. Basic concepts of numerical solution has been described, especially a non-standard way of treatment of process rates based on physical limitations, which ensures that mass is conserved during interphase mass transfer.

The 1D bed model has been implemented into a computer program GRATECAL 1.3 with a graphical user interface. The program can serve for a study of particular processes such as heat-up, drying, pyrolysis and char combustion

independently as well as for any desired combination of processes including a complete simulation of combustion in an experimental reactor.

3 ANALYSIS OF SOME SPECIFIC MODELLING ISSUES

The computer program GRATECAL 1.3, developed within this work, has been used in a series of simulations conducted in order to analyse some specific physical and numerical modelling issues. In the absence of experimental work due to unavailability of a testing rig, the results were interpreted by physical reasoning and, where possible, qualitatively compared to those of other researchers. From these results, recommendations are given regarding mainly the effectivity of simulations and quality of numerical results. Also, an original method for checking the conservativeness of a numerical model by means of additional mass and energy balance calculation is presented. The method is applied to several case studies to demonstrate its capabilities. Finally, a parametric study of effects of convergence criteria on the mass and energy balance of the system is carried out and new findings are summarized.

Wheat straw has been used as a fuel common to all simulations. Setup of input parameters used for particular cases can be found in the author's works [6, 7, 8, 10].

3.1 EFFECTS OF DRYING MODELS

In order to compare the available types of drying models, two models adopted from the literature are used to compute the drying rate, namely the first-order kinetic rate model (2), and the modified diffusion-limited rate model

$$r_{\mathrm{dry}} = Y_{\mathrm{H_2O}} k_{\mathrm{d}} A_{\mathrm{p}} \left(\rho_{\mathrm{H_2O,surf}} - \rho_{\mathrm{H_2O,g}} \right) \qquad [\mathrm{kg/m^3\,s}], \tag{5}$$

where k_{d} [m/s] is coefficient of mass transport by diffusion, A_{p} [$\mathrm{m^2/m^3}$] is volumetric surface of fuel particles and $\rho_{\mathrm{H_2O,surf}}, \rho_{\mathrm{H_2O,g}}$ are densities of water vapour at the particle surface and in the gas flow, respectively.

Figure 8 shows propagation of the drying front along the fuel bed. It can be seen that both models predict almost identical propagation rates. Thus the steady state is reached after the same time as may be easily seen in Figure 9, which shows total mass of solid as a function of time. However, the drying fronts of the two models are different in terms of both intensity and thickness. While the first-order kinetic rate model predicts non-zero drying rate values wherever solids contain any moisture, the diffusion-limited model significantly bounds the zone to much thinner domain. Also maxima of the drying rates differ by one order of magnitude. It is interesting to note the agreement with almost linear mass loss during grate combustion process documented e.g. by Lans et al. [20]. The drying process is clearly rate-limiting also for the combustion process.

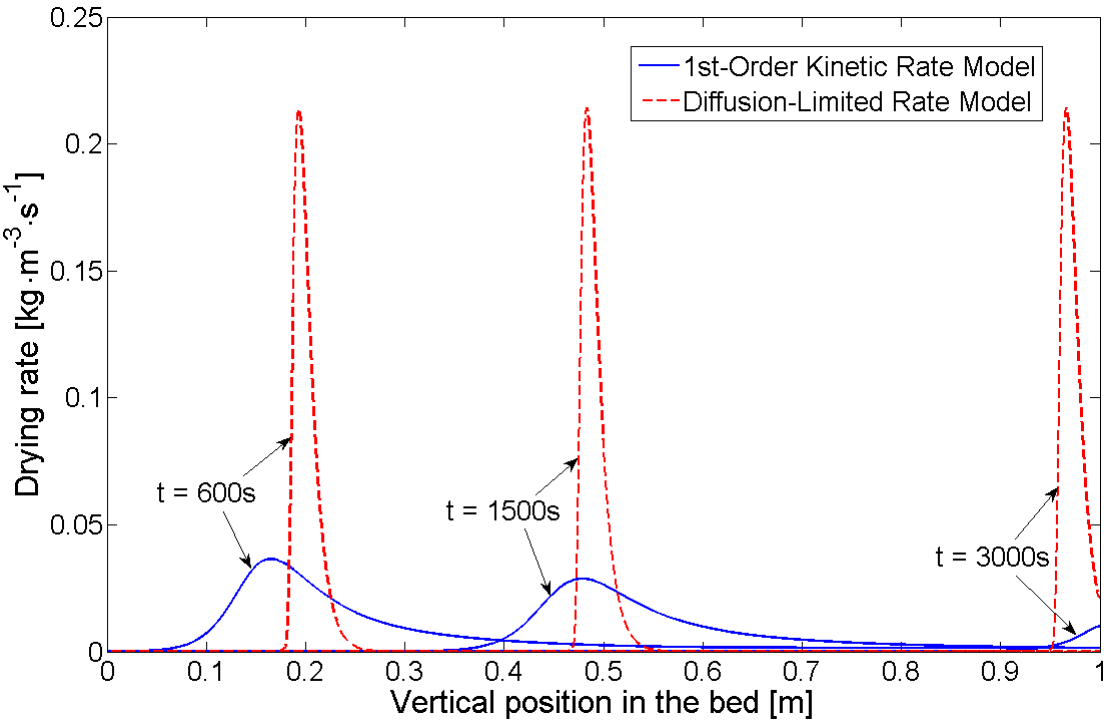

Figure 8: Propagation of drying front as predicted by the first-order kinetic rate model and modified diffusion-limited rate model.

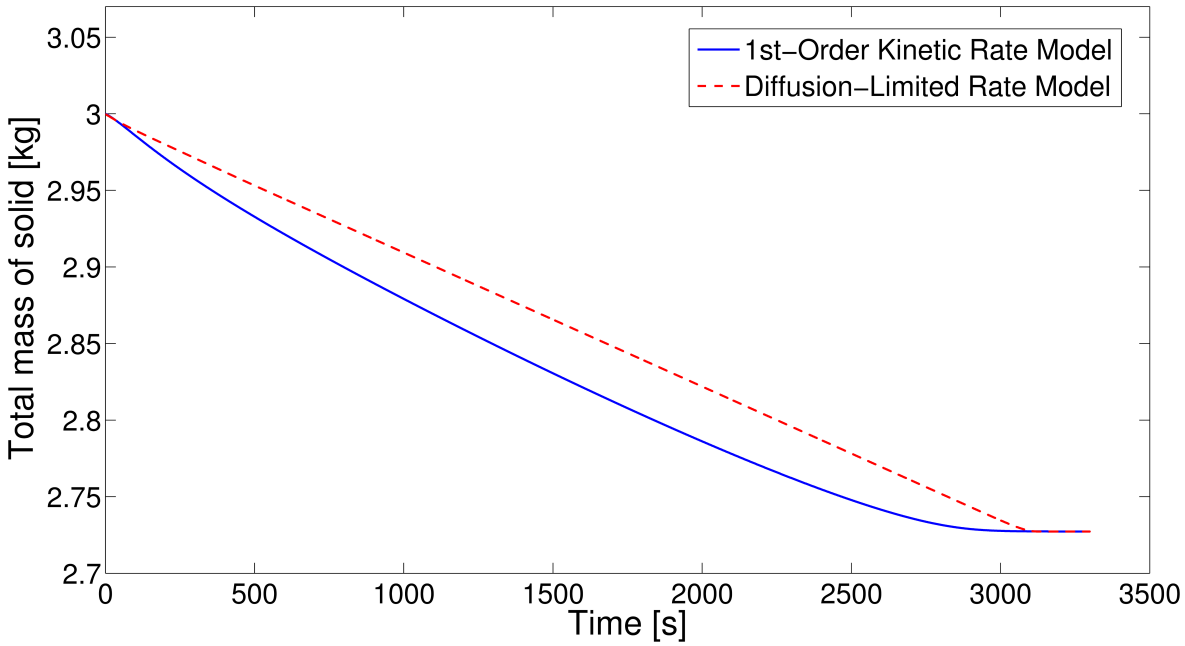

Figure 9: Solid mass loss curves as predicted by the first-order kinetic rate model and modified diffusion-limited rate model.

3.2 EFFECTS OF VARIABLE POROSITY

In order to assess the approach for modelling the change of bed porosity and particle size during wheat straw combustion, several simulations have been performed, three of which are discussed in more detail in this section. The dif-

ference between simulations is in the initial size of a solid particle and whether the change of bed porosity was taken into account or not.

The effects of porosity on burning rate with respect to the primary air flow rate were studied in [20, 24]. At low air flow rates (around 0.1 kg/m^2 s), the burning rate decreases as the bed porosity increases. As for the particle size, larger fuel particles cause lower burning rates, thicker reaction zonse and higher bed temperatures. Figure 10 illustrates propagation of char combustion reaction fronts for a case of particles of the same initial size ($d_p = 4$ mm) as calculated during simulations with constant porosity (solid line) and variable porosity (dash-dotted line). It can be seen in Figure 10, that the reaction front as pre-

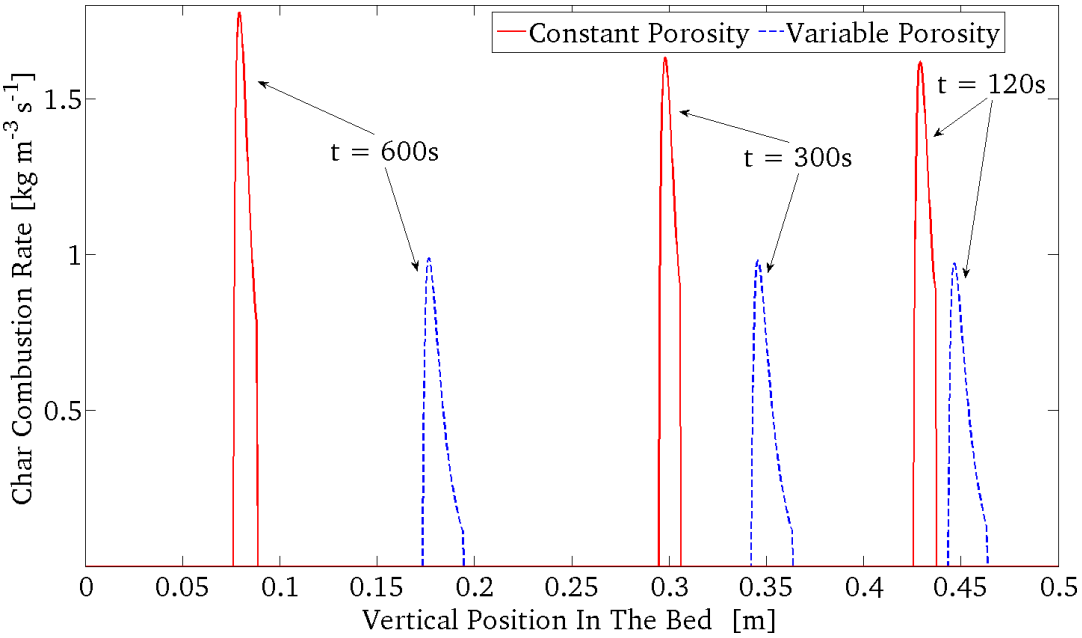

Figure 10: Comparison of propagation of char combustion reaction fronts as predicted by constant- and variable-porosity models.

dicted by the model with variable bed porosity moves downward the bed with lower velocity than the reaction front in case of the constant porosity model. This corresponds with the aforementioned results of other authors, because the bed porosity increases during straw combustion. The value of the char combustion reaction rate predicted by the variable-porosity model is lower than the value obtained by the constant-porosity model, because volumetric surface of particles decreases with increasing porosity. Figure 11 shows propagation of reaction front in the bed of particles with $d_p = 20$ mm. The variable-porosity model has been used. The reaction front travels down with considerably lower speed than in the bed of 4-mmparticles. A thicker reaction zone can be seen as well. This corresponds well with experimental results ([23, 24]). However, a thicker reaction zone can also be seen in the case of 4-mm particles for the variable-porosity compared to the reaction zone from the simulation with the

constant-porosity model (Figure 10). This unexpected behavior can be caused by low volumetric surface of particles, which in turn has impact on the inter-phase heat transfer. Fuel particles shrink during the combustion, but in fact the effect is the same as in case of large particles, which is in contradiction. To remedy this effect, internal particle porosity should be considered.

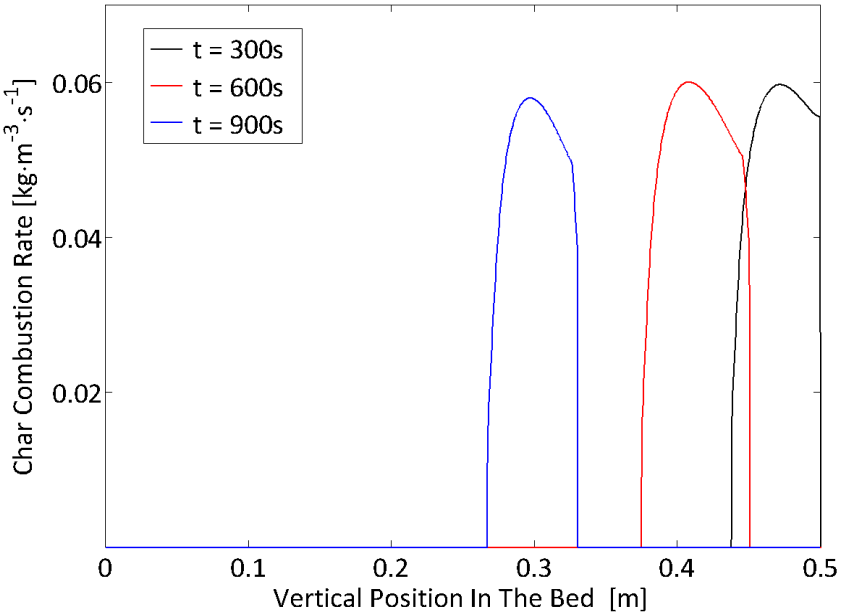

Figure 11: Propagation of char combustion reaction front as predicted by the variable-porosity model for 20-mm particles.

3.3 BALANCE-BASED CONTROL OF THE CONSERVATIVENESS

A balance-based control method has been proposed and implemented to check the conservativeness of the 1D transient bed model. A balance equation for a conserved quantity ϕ in a control volume can generally be written as

$$\phi^{f} - \phi^{i} + \phi^{\text{out}} - \phi^{\text{in}} = 0. \tag{6}$$

where superscripts i and f denote initial and final conditions and terms ϕ^{in}, ϕ^{out} the amounts of the quantity ϕ flowing into and out of the control volume, respectively. While initial conditions are given explicitly, the terms ϕ^{in}, ϕ^{out} are usually unknown functions of time and therefore must be calculated at the end of each time step. Equation (6) is not satisfied exactly due to various errors [2]. Therefore, a residual R_{bal} of the balance equation and the relative imbalance I_r are defined as

$$R_{\text{bal}} = \phi^{\text{f}} - \phi^{\text{i}} + \phi^{\text{out}} - \phi^{\text{in}}, \tag{7}$$

$$I_{\text{r}} = \frac{|R_{\text{bal}}|}{\phi^{\text{i}} + \phi^{\text{in}}}. \tag{8}$$

Mass and energy balance equations for the 1D model can be derived from Equation (6). Initial and final mass contents of the bed are given by mass of the fuel and gas occupying voids of the bed. In a batch mode of combustion, mass flowing into and out of the packed bed is determined from primary combustion air and flue gas leaving the bed, which is obtained at the end of each time step when iterations converge. Energy balance equation is given by analogous equations, which take into account the lower heating value (LHV) and sensible heat of both fuel and gas. In addition, energy transmitted by radiation between the top of the bed and over-bed environment must be included in the balance as well.

At the end of each time step, also unscaled residuals [3] of discretized mass and energy transport equations are stored. The sum of the residuals over simulated time will give total mass and energy residuals as an estimate of the upper bound of the overall error. When the simulation is finished, mass and energy content of gas and fuel left in the reactor is computed. Overall mass and energy imbalances are evaluated and compared to values of total residuals of discretized mass and energy transport equations as a measure of imperfect conservation. If either of imbalances is not covered by the corresponding total residual, then the bed model does not conserve the physical quantity and contains an error.

The balance-based control method has been used to verify correctness of the GRATECAL 1.3 code implementation in two test studies, which have revealed certain errors in the definition of source terms in models adopted from literature as discussed in the previous chapter.

3.4 EFFECTS OF CONVERGENCE CRITERIA

The balance-based method has been used to analyse effects of convergence criteria on mass and energy imbalance of the modelled system. Such an investigation is motivated by the fact, that the system of governing equations is solved by an iterative procedure and iterations are continued until convergence criteria are met. However, whenever a process is stopped not reaching its limiting value, a truncation error is introduced, so the incomplete convergence generates mass and energy imbalance in the system. This effect becomes more important in unsteady simulations, in which truncation errors cumulate at the end of each time step. Another reason to carry out this kind of parametric study is to determine *a sufficiently small value* of the relative error for judging the convergence, which, otherwise, is not specified in literature on general iterative numerical methods and depends on the nature of the solved problem.

The effect of convergence criteria on mass and energy balances is studied through a series of simulations of heat-up and pyrolysis as essential stages of combustion of dry wheat straw in an experimental fixed-bed reactor. Since com-

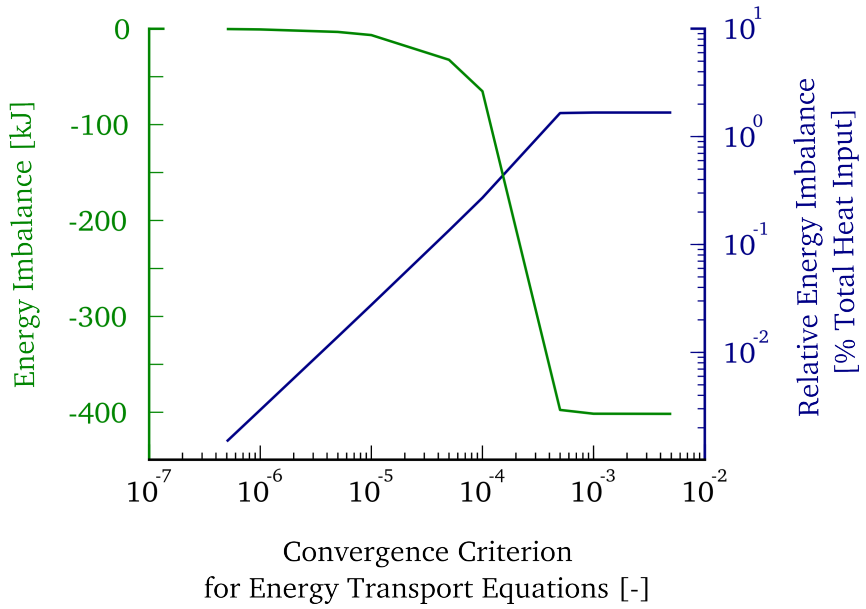

Figure 12: Total and relative energy imbalances as obtained by simulations of heat-up of dried wheat straw by preheated primary air (398 K) and over-bed radiation.

bustible volatiles are released during pyrolysis, even a small mass imbalance in the system can lead to large errors in the energy conservation. Values of scaled residuals as convergence criteria are varied in the interval $\left(10^{-7}, 10^{-2}\right)$ with a step of a half of an order.

The effect of scaled residuals for energy transport equations on the energy imbalance during heat-up of wheat straw by primary air (398 K) and over-bed radiation is shown in Figure 12. The convergence criterion for gas species transport equations is fixed to 10^{-3}. It can be seen that the energy imbalance significantly increases for values of energy scaled residual greater than 10^{-5} and keeps very low for values less than or equal to 10^{-6}, which is the default value for the energy equation in ANSYS FLUENT [3].

However, the value 10^{-3} of scaled residuals for gas species transport equations seems to be too low to obtain sufficiently low energy imbalance after volatile matter (approximately 1.1 kg, 79.28wt% on dry basis) is completely pyrolysed as shown in Figure 13. Although the convergence criterion for energy transport equations is fixed to 10^{-6}, mass imbalance produces relativelly large energy imbalance as long as scaled residuals are greater than 10^{-6}. In order to obtain sufficiently accurate results from in-bed simulations in terms of mass and energy conservation within the packed bed, it is, therefore, suggested to require all the scaled residuals to drop to as low as 10^{-6} or lower.

3.5 INVERSE APPLICATION OF THE BALANCE METHOD

The presented method offers an alternative to setting of convergence criteria, which is interesting from practical point of view. Instead of defining scaled resid-

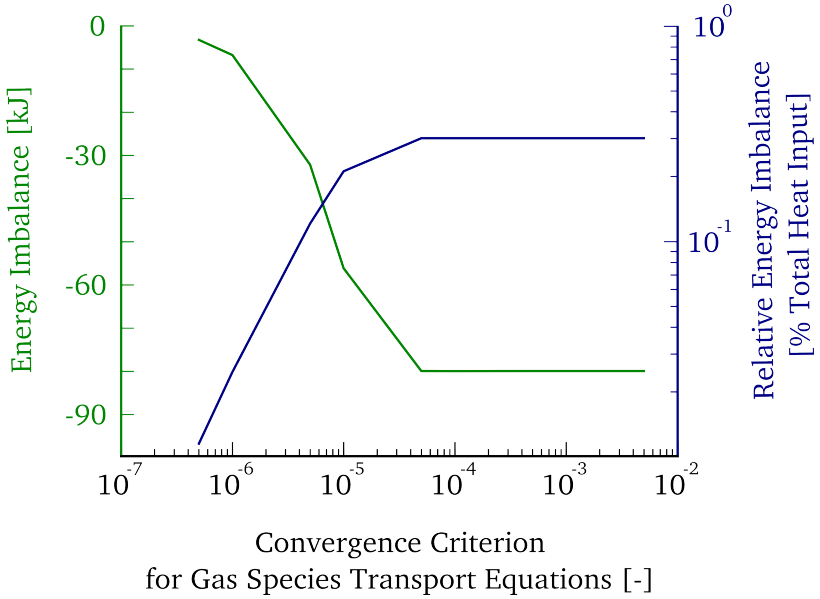

Figure 13: Total and relative energy imbalances as obtained by simulations of pyrolysis of dried wheat straw by preheated primary air (698 K) and over-bed radiation.

uals, the convergence criteria could be set in terms of the total mass and energy imbalance of the system. Such a requirement is somehow more natural than a drop of a nondimensional quantity, as the error is defined by physical quantities, that are commonly used in engineering analyses. However, the physical limits would have to be set very carefully, since too strict requirement on the magnitude of imbalance might lead to undesirable long computational times due to very low equivalent scaled residuals. For this purpose, more accurate discretization methods and fast converging iterative schemes would have to be used or developed in order to achieve low imbalances in reasonable computational times.

3.6 SUMMARY

The capability of the simulation tool has been demonstrated on a series of simulations. Among the physical issues considered, analysis of propagation of drying and combustion reaction fronts in the bed of wheat straw particles have been done. Results from simulations qualitatively agree with data available in literature. It has been suggested to include modelling of particle internal porosity in order to obtain correct reaction zone thickness, if porosity of the bed is allowed to change during combustion.

In order to check the conservativeness of the bed model, mass and energy balance method has been implemented in the code providing for detailed analysis of various errors arrising during a simulation. The method has revealed certain errors in the definition of source terms in models adopted from literature. This has been done to reconcile the base model to yield a conservative model. A

parametric study of the effects of convergence criteria on total mass and energy imbalance of the system has been carried out. From the results, it has been suggested to set the criteria on the scaled residuals for all variables to 10^{-6} or lower in order to obtain acceptably low mass and energy imbalance. A possible inverse use of the balance method is also outlined.

4 C LIBRARY OF FUNCTIONS FOR COUPLED BED-FREEBOARD MODELLING IN ANSYS FLUENT

The capabilities of the commercial CFD software ANSYS FLUENT can be extended by use of the so-called user defined functions (UDF), which allow a user to define custom models or modify the existing ones, making it even more flexible. By means of UDF's, a bed model can be coupled with a freeboard model, so that heat and mass fluxes leaving the bed form the inlet boundary conditions for the freeboard, while radiation heat flux obtained from the solution of the freeboard can be passed onto the bed model. If this procedure is repeated iteratively, converged solutions of both models can be reached, when the radiation heat flux ceases to fluctuate.

In order to couple the developed bed model with a freeboard model, a C source code has been generated from the MATLAB source codes of GRATECAL and a UDF has been programmed to pass data from the in-bed simulations to the freeboard model as boundary conditions at the furnace inlet.

4.1 DESCRIPTION OF COUPLED MODELLING METHODOLOGY

The coupled methodology is based on the idea, that a fuel bed can be 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.

The plane of a grate is chosen as the interface in the first stage of coupled models development as it provides a convenient way to realize the coupling. Also the radiation heat transfer at the bed top is simplified such that a temperature profile along the bed length for calculation of the heat flux is predefined and set constant. Therefore, the current version of the interface provides for a one-way coupling only.

4.2 WORKING WITH UDF

Following the walking-column approach, both duration of the simulation and time steps are no longer set by a user, but determined from geometry and mesh

properties of the grate such that $t = L_G/v_G$ [s], where L_G [m] is the grate length and the time step is $\Delta t = t/N_f$, where N_f is the number of faces, that discretize the grate along its length. If a computed time step exceeds 0.5 s, then the code finds a number $n_{\Delta t} > 1$ such that $\Delta t/n_{\Delta t} \leq 0.5 < \Delta t/(n_{\Delta t} - 1)$, so that a solution for each face is obtained in $n_{\Delta t}$ time sub-steps to ensure numerical stability. Velocity and length of the grate as well as the number of faces is passed to the main function from ANSYS FLUENT in a structure `fluentDataStruct`.

Also an information on the orientation of the grate with respect to the coordinate system must be provided in order to properly match transient solutions with corresponding faces. It is assumed, that the furnace is oriented such that the grate declines in a direction of one of the coordinate axes (if the grate is not inclined, then the direction from the feeder to the ashpit must correspond with either of coordinate axes direction). The axes x, y, z are denoted by numbers $0, 1, 2$, respectively.

In summary, parameters needed to describe the grate for the purpose of matching transient solutions to proper correct positions on the grate, are as follows:

- Boundary zone ID's.
- Velocity of the grate v_G [m/s].
- ID number of the coordinate axis, along which the grate declines. ID numbers are assigned to axes as follows: $0 \rightarrow x, 1 \rightarrow y, 2 \rightarrow z$.

These parameters must be provided by a user in the file `fluentData.h`.

The main source code file of the UDF is `udf_gc1D.c`, which contains several `DEFINE` macros and a number of functions, that are called by macros in order to initialize data and process results from GRATECAL to set profiles of boundary conditions. A user first must set the main descriptive parameters of the grate in `fluentData.h`. In the same file, a valid full path to the file `gcData.txt`, that contains information on settings of GRATECAL including gas and fuel properties etc., must be provided. The default total number of gas species in the simulation must not be changed.

Three `DEFINE_PROFILE` macros are available in the UDF, by means of which boundary conditions can be modified. Note, that the UDF for boundary conditions for all variables must be defined. These include:

- `udf inlet_species` for all gas species. Gas species may be ordered in the list of mixture arbitrarily provided, that N_2 is the last item in the list.
- `udf inlet_m_flux` for mass flux in units of [kg/m^2 s].
- `udf inlet_temp` for gas temperature.

4.3 SUMMARY

Using MATLAB Coder, a C code has been generated from MATLAB source files of GRATECAL 1.3 in order to use the program as a tool for calculation of the boundary conditions at the grate (inlet) by means of UDF in ANSYS FLUENT. An interface for coupling the bed and freeaboard models has been developed and implemented into a library of C-functions as a UDF, which can be loaded into ANSYS FLUENT to set and modify boundary conditions at the furnace inlet, providing for a one-way coupling of the two models. The UDF can be used for a wide range of grate furnace CFD models.

5 CONCLUSIONS

The present work is concerned with numerical modelling of grate combustion of solid fuels, especially biomass and municipal solid waste. The scope of investigated topics is restricted to modelling of processes, that take place within a fuel bed on a grate, as knowledge of the process dynamics in the bed is essential for optimization and development of grate-firing techologies. This is emphasized by the fact that results from CDF simulations of grate combustion depend on the quality of input data including information on temperature, mass flux and chemical composition of flue gas leaving the bed. Therefore, the attention is turned to development of a reliable numerical model of packed-bed combustion as it may help improve both results from simulations and knowledge of principles of solid fuel combustion in fixed or moving beds.

Based on a review of existing bed models, a one-dimensional transient heterogeneous numerical model of combustion in an experimental reactor has been developed. The model has been implemented into a computer program called GRATECAL 1.3. The program solves governing equations numerically by the finite volume method. A special numerical treatment of process rates based on physical limitations has been introduced, which ensures that mass is conserved during interphase mass transfer. It also has been noted, that interpolation of velocity-dependent diffusion terms to control volume faces using an arithmetic mean slows down the convergence. Such a term should be interpolated using an upwind scheme.

A method for control of mass and energy balance over the system has been developed, by means of which the model can be checked and corrected for errors to yield a conservative model. The method has been applied to a series of case studies, which have revealed certain errors in definitions of mass source terms, so that data adopted from literature have been reconciled. The model has been used in analysis of propagation of drying and char combustion reaction fronts, demonstrating the capabilities of the developed simulation tool. A parametric study on effects of convergence criteria on total mass and energy imbalance of the system due to incomplete convergence has been carried out. It has been

concluded that all the scaled residuals must drop to as low as 10^{-6} or lower in order to obtain sufficiently accurate results from in-bed simulations in terms of mass and energy conservation within the packed bed.

The second part of the work has been devoted to implementation of an interface, through which the bed model can be coupled with the freeboard model created in ANSYS FLUENT. Using MATLAB Coder, a C code has been generated first from MATLAB source files. Then, the interface has been programmed in C programming language and implemented as a user defined function, that can be loaded into ANSYS FLUENT to set boundary conditions at the furnace inlet at an iteration. The UDF provides for a one-way coupling of the two computational models. The interface is general enough to be used for a wide range of models of grate furnaces.

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Abstract

The present work is focused on numerical modelling of grate combustion of solid fuels by means of computational fluid dynamics (CFD) methods. A one-dimensional transient numerical model of combustion in an experimental reactor is developed and implemented into a computer program called GRATECAL 1.3. A method for control of mass and energy balance over the system is developed and applied to a series of case studies, which have revealed certain errors in definitions of mass source terms, so that data adopted from literature have been reconciled.

The model is used for analysis of propagation of drying and char combustion reaction fronts in a bed of wheat straw particles. It is suggested to include modelling of particle internal porosity change in order to obtain correct reaction zone thickness, if porosity of the bed is allowed to change during combustion. The balance-based method is also used to analyse effects of convergence criteria on mass and energy imbalance of the modelled system. It is found that all the scaled residuals must drop to as low as 10^{-6} or lower in order to obtain sufficiently accurate results from in-bed simulations in terms of mass and energy conservation within the packed bed.

The second part of the work is devoted to development of a library of user-defined functions for the commercial CFD software ANSYS FLUENT for coupling the bed model with a freeboard model of a real combustion unit in order to specify the boundary conditions indirectly using results from in-bed simulations. The created interface is general enough to be used for a wide range of models of grate furnaces.

Abstrakt

Předkládaná práce je zaměřena na numerické modelování spalování tuhých paliv na roštu metodami výpočtové dynamiky tekutin (CFD). V rámci práce byl vyvinut jednorozměrný nestacionární model spalování v experimentálním reaktoru a implementován do počítačového programu GRATECAL 1.3 včetně grafického uživatelského rozhraní. Byla vyvinuta metoda pro kontrolu hmotnostní a energetické bilance systému a následně aplikována v řadě studií, v rámci nichž byly odhaleny některé chyby týkající se definic zdrojových členů, které byly převzaty z literatury a opraveny.

Pomocí modelu byla provedena analýza šíření čela sušení a reakce hoření koksu po výšce lože pšeničné slámy. Na základě výsledků těchto analýz bylo doporučeno zahrnout i modelování změny porozity částic paliva, aby šířka reakční zóny byla predikována korektně v případě, že je uvažována změna porozity celého lože. Rovněž vyvinutá bilanční metoda byla použita k analýze vlivu kritérií konvergence na hmotnostní a energetickou nerovnováhu simulovaného systému. Bylo zjištěno, že škálovaná rezidua rovnic všech veličin by měla pok-

lesnout aspoň na hodnotu 10^{-6}, aby bylo dosaženo nízké hmotnostní a energetické nerovnováhy a tudíž uspokojivě přesných výsledků ze simulací v loži.

Druhá část práce je věnována vývoji a implementaci knihovny uživatelem definovaných funkcí pro komerční CFD nástroj ANSYS FLUENT, které umožňují propojit model lože s modelem komory reálné spalovací jednotky, aby byla umožněna dynamická změna okrajových podmínek na vstupu do komory v závislosti na výstupech ze simulací v loži. Vytvořené rozhraní pro propojení těchto dvou modelů je dostatečně obecné pro aplikaci na širokou škálu modelů roštových kotlů.