



# Modelling wood combustion under fixed bed conditions<sup>☆</sup>

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## Abstract

A computer model describing the conversion of wood under packed-bed conditions is presented. The packed bed is considered to be an arrangement of a finite number of particles, typically sized between 5 and 25 mm, with a void space left between them. Each particle is undergoing a thermal conversion process, which is described by a one-dimensional and transient model.

Within the single-particle model, heating, drying, pyrolysis, gasification and combustion are considered, whereby each particle exchanges energy due to conduction and radiation with its neighbours. Because of the one-dimensional discretization of the particles, heat transfer and mass transfer is taken into account explicitly. Therefore, no macrokinetic data are needed within the model. For ease of implementation and access, kinetic data and property data are stored in a database. The global conversion of the packed bed is represented by the contributions of single particles, where each particle is coupled to the surrounding gas phase by heat and mass transfer. For gas phase flow through the porous bed, the conservation equations for mass, momentum and energy are solved on a Cartesian mesh by a Finite Volume method.

Experiments have been performed to validate the single particle model for the conversion of beech wood during pyrolysis and char combustion. Agreement between experimental and predictions obtained by the model is very satisfactory. However, for wet wood, changes in structure seem to enhance the heat transfer to the solid which is not yet covered in the model.

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## 1. Introduction

An increasing use of renewable energy sources, such as wood, is an important issue in a future energy market to solve the CO<sub>2</sub> problem. Most automatic furnaces used in wood combustion are understoker and grate furnaces, in which the fuel is converted in a packed bed and the combustion process is completed in the furnace chamber. In recent years, progress has been achieved in the optimisation of furnaces with respect to reduced emissions and higher efficiencies. However, further improvement requires detailed knowledge of the combustion process in the furnace.

For the optimisation of flow conditions in combustion chambers, computational fluid dynamics (CFD) have become a useful tool, employed together with experiments. While for investigation of the flow conditions in the gas phase

commercial CFD codes can be applied, the prediction of solid fuel conversion into raw gas in the packed bed is difficult.

Therefore, a model is required which can predict the influence of operational parameters on solid fuel conversion, in such a way that the boundary conditions to gas phase simulation by a CFD code can be calculated.

Several approaches predicting the solids conversion rate in packed beds, or the species distribution in the raw gas are presented in the literature. Ford et al. [1] described a model of the conversion of coal on a grate which is based on the assumption of a combustion regime fully controlled by boundary layer diffusion. No further description of the flow in the bed is taken into account. To predict the velocity of the burning front in a bed of wood particles, Fatehi and Kaviany [2] developed a model based on equilibrium assumptions. Raupenstrauch [3] coupled a model to calculate solids conversion by a CFD code which predicted the steady state flow through the porous bed. Particle mass is coupled to its size by a simplified approach but no discretization of the particle's dimension is applied. A transient heterogeneous model of packed beds was developed by Hartner [4], with

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Nomenclature			
$A$	Area ( $\text{m}^2$ )	$\Gamma$	diffusion coefficient
$a_i$	Interpolation function coefficients	$\varepsilon_p$	porosity (–)
$c$	gas concentration ( $\text{mol}/\text{m}^3$ )	$\lambda$	thermal conductivity ( $\text{W}/\text{mK}$ )
$c_v$	specific heat ( $\text{J}/\text{kg K}$ )	$\mu$	dynamic viscosity ( $\text{kg}/\text{m s}$ )
$D$	diffusion coefficient ( $\text{m}^2/\text{s}$ )	$\rho$	density ( $\text{kg}/\text{m}^3$ )
$E_a$	activation energy ( $\text{kJ}/\text{mol}$ )	$\omega$	source term
$F_{i \rightarrow j}$	view factor	$\bar{\omega}$	averaged source term
$k_0$	frequency factor ( $1/\text{s}$ )	$\langle \rangle$	average value in porous media
$K$	permeability ( $\text{m}^2$ )		
$\dot{m}$	mass flow ( $\text{kg}/\text{s}$ )	<i>Indices</i>	
$n$	shape factor (0 for plate, 1 for cylinder, 2 for sphere)	b	bed
$\dot{q}$	heat flux ( $\text{W}/\text{m}^2$ )	c	contact
$\dot{r}$	reaction rate ( $\text{mol}/\text{m}^3 \text{ s}$ )	ch	chemical reactions
$R$	gas constant ( $\text{J}/\text{mol K}$ )	cond	conduction
$t$	time (s)	conv	convection
$\Delta t$	outer integration step (s)	E	east face of volume element
$T$	temperature (K)	eff	effective
$u$	gas velocity in the particle (m/s)	h	heating
$u$	mass of water/mass of dry fuel	i	inner
$v$	gas velocity in the bed (m/s)	pa	particle
$Y_i$	species mass fraction	rad	radiation
$\alpha$	heat transfer coefficient ( $\text{W}/\text{m}^2 \text{ K}$ )	s	value at the surface
$\beta$	mass transfer coefficient (m/s)	th	thermal
$\gamma$	contact angle ( $^\circ$ )	w	dry wood
		$\infty$	value in the bulk flow

the solid fuel reactor discretized in one-dimension. Beckmann and Scholz [5] divided the bed of a grate furnace into various zones, each of them represented by a perfectly stirred reactor to describe char conversion on a grate. Mixing due to motion on the grate can be accounted for by the mass exchange between the reactors. Based on laboratory reactor experiments Kuo [6] applied empirical correlations predicting typical design parameters, such as grate burning rate and volume load for the combustion of wood in packed beds. Goh et al. [7] developed a model based on different zones for virgin, dried and pyrolysed fuel and ash to calculate the boundary conditions for a CFD code. Describing the fuel conversion requires macrokinetic data. Investigating simultaneous drying and pyrolysis of a packed bed of wood particles, Saastamoinen and Haukka [8] presented a one-dimensional model, where drying and pyrolysis are solved on a single particle with the vaporisation taking place on a shrinking core. For comparisons with experimental results at a laboratory furnace, Shin and Choi [9] recently discussed a one-dimensional transient model for the conversion of waste particles on a grate. Using a finite volume approach global kinetic data are applied to solids conversion in a volume element assuming kinetic control of the process.

Most of the models are restricted to a certain part of the conversion process or require empirical information, thus limiting application to a specific case for which the data are

valid. Therefore the aim of the present work is to develop a general model covering the entire conversion process of biomass fuels, from drying to char conversion, which can be used to determine rate limiting conditions and potentials for optimisation in packed-bed combustion. Modelling the packed bed as a porous media, as often presented in literature, macrokinetic or empirical data is required to capture the influence of particle size on the conversion. Thus, to reduce the need of empirical data, a different approach needs to be chosen here.

## 2. Modelling thermal conversion of a packed-bed

### 2.1. Single-particle model

In wood furnaces, the packed bed consists of particles of a large variety of sizes, typically sized between 5 and 25 mm for automatic furnaces. During the thermal conversion of wood, different processes such as drying, pyrolysis and char conversion, occur which may overlap to some extent within a particle depending, e.g. on fuel type, particle size or heating rate. It is not feasible to determine macrokinetic data for all the different conditions which can prevail within a packed bed. To apply kinetic data derived from dust samples under the assumption of kinetic control of the conversion process to

larger particles, heat and mass transfer within the particle need to be taken into account [10]. Therefore, spatial discretization is required, when describing the conversion process of a single fuel particle. However, as the formulation for a single particle is part of an overall packed-bed model, the numerical effort which can be spent on this subprocess is limited. As a compromise between computation time and accuracy of description, a transient one-dimensional model is employed to predict the conversion process in each particle. In the literature, models are discussed for simulating one or two sub-processes such as pyrolysis or char combustion of single wood particles among the overall process [11–14]. Here, the whole process, including drying, pyrolysis, char combustion and gasification, is incorporated in the authors' model. The governing equations describing the conservation of a scalar  $\phi$  versus the radius of a solid particle are implemented in a general form with the exponent  $n$  in Eq. (1), representing the formula for an infinite plate, an infinite cylinder and a sphere for  $n = 0, 1, 2$ .

$$\frac{\partial}{\partial t} \langle \rho \rangle \langle \phi \rangle = \frac{1}{r^n} \frac{\partial}{\partial r} \left( \Gamma_{\text{eff}} r^n \frac{\partial}{\partial r} \langle \rho \rangle \langle \phi \rangle - r^n \langle \rho \rangle u \langle \phi \rangle \right) + \omega \quad (1)$$

Each property value in a volume element of the porous particle is calculated as an average over the values of the species currently present in the control volume. The equations are discretized in space by a finite volume approach with the values for energy and species averaged over a control volume assuming thermal equilibrium between the solid and the gas phases within the porous particle. The processes in the particle are influenced by diffusion and convection associated with chemical reactions. During drying and pyrolysis, the convective terms play an important role, because of the humidity and the volatiles content of the wood, whereas char combustion and gasification are determined by diffusion. For the effective thermal conductivity the contribution of radiation in the pores of the particle according to Ref. [12] is included additionally to the property data.

The solution of the momentum equation to calculate the flow velocity of the gases in the porous particle would exceed the numerical effort acceptable for a single particle as part of a packed-bed model. Therefore, a simplified approach predicting the flow velocity is applied. The flow within the particle is assumed to be determined by the gas production rate due to solids conversion. Thus, the continuity equation can be applied to predict the velocity, always assuming an outward flow from the particle. Under the assumption that the change of the source terms  $\omega_G$  due to gas production at different positions in the particle is much slower than the propagation of the pressure wave in the solid, the flow velocity on the boundary face of a volume element can be calculated by Eq. (2), where  $\omega_{G,j}$  stands for the gas source terms in the inner elements with respect to the boundary face of the volume element  $i$ .

$$u_i = \frac{\sum_{j=1}^n \omega_{G,j}}{A_{i,E} \langle \rho_{G,i} \rangle} \quad (2)$$

*Boundary conditions.* Boundary conditions are required to complete the system of equations. At the centre of the fuel particle, all gradients are set equal to zero. At the particle surface, heat is transferred between the fuel particle and the surrounding gas phase under the impact of convection. Moreover heat transfer to and from the particle occurs as a result of conduction and radiation between the solid particles, which will be discussed below. Thus, the energy at the outer shell can be balanced according to Eq. (3).

$$-\lambda_{\text{eff}} \frac{\partial \langle T \rangle}{\partial r} \Big|_{r=R} = \alpha (\langle T_R \rangle - T_{\infty}) + \dot{q}_{\text{rad}} + \dot{q}_{\text{cond}} \quad (3)$$

Within the packed bed, the heat transfer coefficient is based on an empirical correlation accounting for an increase in heat transfer relative to a single particle in a gas flow according to Ref. [14]. Thus, calculation of the Nusselt number in the bed  $\text{Nu}_b$  bases on the Nusselt number of a single particle in a gas flow  $\text{Nu}_{\text{pa}}$ , as stated in Eq. (4)

$$\text{Nu}_b = 1 + 1.5(1 - \varepsilon_p) \text{Nu}_{\text{pa}} \quad (4)$$

Calculated values of the heat transfer coefficient based on this approach are in good agreement with experimental values measured in a packed bed of wood particles [15], even if the Reynolds numbers in packed bed combustion are quite low.

The boundary conditions for mass transfer at the particle surface are given by

$$-D_{\text{eff}} \frac{\partial \langle c_i \rangle}{\partial r} \Big|_{r=R} = \beta_i (\langle c_{R,i} \rangle - c_{\infty,i}) \quad (5)$$

where  $\langle c_{R,i} \rangle$  refers to the molar concentration of the species  $i$  at the surface and  $c_{\infty,i}$  indicates concentration in the bulk flow. The calculation of the mass transfer coefficient bases on the Sherwood number calculated in the same way as the Nusselt number in Eq. (4). Gas flow out of the particle reduces the transfer coefficients; thus, Stefan's correction is introduced to the calculation of the coefficients.

*Chemical reactions.* The efficient description of the chemical source term requires a general approach, able to treat pyrolysis, char conversion or homogeneous reactions. Each conversion process consists of one or more reactions describing the degradation from the educts to the products. Each reaction then is represented by a maximum number of three educts and three products, with the temperature dependence of the rate for reaction  $i$  described by the Arrhenius equation in the following form, Eq. (6).

$$\dot{r}_i = k_0 \exp\left(-\frac{E_a}{RT}\right) \prod_{k=1}^3 c_{i,k} \quad (6)$$

The computer program allows different models for the conversion of wood or char to be selected from a database [16] supplying the corresponding set of chemical reactions which occur in a particle. This approach allows the influence of different models and parameters on the conversion to be investigated easily. The database is linked to the code,

allowing the data to be changed without modifications of the computer code describing the actual problem.

As has been discussed in the literature, the drying process in wood can also be described by a heterogeneous reaction [3,17]. However, comparisons between experimental and calculated data showed, that the pseudokinetic data would have to be adapted to the given boundary conditions, which excludes this model from general use. Therefore, drying is solved via a constant evaporation temperature, on the assumption that, above this temperature, all energy will be consumed by the drying process as long as water remains in a control volume of the particle. This approach guarantees that no water evaporates below the evaporation temperature and temperature in the drying section remains constant. This matches the experimental observation made by Ref. [18] for wet coal particles.

Heterogeneous reactions during char conversion can be represented in the form of Eq. (6) or as intrinsic rates by replacing the molar concentration of the solid species by the specific surface. Whether or not a reaction rate is handled as an intrinsic rate is indicated by the database; so, no changes need to be made in the computation code. More detailed models for the description of heterogeneous reactions would exceed the numerical effort which is acceptable for the single-particle model. Moreover, more detailed models lead to a higher number of parameters which are either unknown or uncertain for char particles from wood pyrolysis, thus the accuracy of description would not be increased necessarily.

Homogeneous reactions within the particle are neglected for the cases presented here. Calculations showed, that in the diameter and temperature ranges of the single particle experiments, less than 10% of the primary tars are converted in the particle by secondary reactions and that char combustion is limited by the amount of oxygen on the particle surface.

*Particle shrinking.* While wood contains only a negligible amount of ash, fuel particles shrink during char combustion, which represents a moving boundary for the solution of the transport equations. Therefore, they are solved in a dimensionless form, allowing an adaptation of the discretization mesh onto the actual particle size. An interpolation function is used to approximate the discrete solution values to obtain the continuous solution versus particle radius. The distribution of the different scalars  $\phi_i$  is characterised by a front moving through the particle. Thus, the following form of the interpolation function is suggested to capture the steep gradients

$$\phi_i(r) = a_0 + a_1[2 + \tanh(a_2r + a_3) - \tanh(a_2r + a_3) + a_4[2 + \tanh(a_5r - a_6) - \tanh(a_5r + a_6)] \quad (7)$$

The coefficients  $a_i$  for the interpolation function (7) are calculated by a least-squares method. If shrinking occurs after an integration step due to depletion of the solid in an outer control volume, the mesh is adapted to the new radius and the discrete values on the mesh nodes are calculated by

the interpolation function with the new radius. Thus, the whole range of char combustion from reacting core mode to shrinking core mode is covered by the model. During drying and pyrolysis the diameter is assumed to remain constant.

*Mathematical solution.* In discretizing the governing equations by a finite volume approach, the partial differential Eq. (1) are transferred into a system of ordinary differential equations (ODE). Because of the different time scales, the resulting ODE system is stiff, requiring a sophisticated integration method to assure stability and accuracy. As a result of several tests [19] a backward differentiation formulae (BDF) proved to be reliable in this instance. Due to the fact that the single particle model is combined with an overlying bed model the integration time step is divided into outer steps for which the submodels, single particle and gas phase, are calculated consecutively and inner time steps of the BDF scheme for the particle model. This reduces the computational effort by shifting calculation procedures to the explicit loop which do not change the values of the single particle significantly within the inner steps. Here, flow velocities of the gases in the particle, property data, the drying process, and particle shrinking are calculated within the explicit loop. This enables the explicit formulation of the ODE problem over each outer time step which helps to increase stability and the convergence rate of the integration process. Moreover, this approach allows to handle the delta function introduced into the system of differential equations to calculate the drying rate at a constant evaporation temperature, as mentioned above.

## 2.2. Packed-bed model

A packed bed in the current application is considered to consist of a finite number of particles with the above-mentioned particle model applied to each particle. The particle is coupled to the surrounding gas phase by source terms, e.g. heat and mass transfer. For the presented case, particles are assumed spherical as regarding discretization and solution of the transport equations.

Due to the arrangement of particles in a packed bed, they form a void space, through which the combustion air flows. The flow through the bed of particles can be described as flow through a porous media with the solid volume taken up by the particles and determining the locally varying porosity. The position of the solid particles may change during the conversion process, because of depletion of solid and shrinkage of the particles. Even if coupling to a motion model based on an overall sum total of forces [20] is intended for the future, a simplified approach is used here. Assuming a constant porosity and a certain number of neighbour particles, the bed mesh is filled up with the solid particles, until the given porosity is reached for the bed cells. If shrinking of the particles occurs, the distribution of particles in the bed is recomputed. This implies a decreasing

bed height with further shrinkage or depletion of the particles and increasing porosity of the upper fluid cells.

A finite volume approach using a Cartesian mesh is applied to discretize the transport equations for species, momentum and energy to which the solid phase contributes source terms due to heat and mass transfer. Within the voids of the bed, diffusion processes are neglected relative to the convective transport. Thus the change of the mass fraction  $Y_i$  for the species  $i$  can be determined by the divergence of the species field and the source term due to the interaction with the solid phase and reactions in the void space of the bed as follows Eq. (8). The source term  $\bar{\omega}_m$  is averaged over the outer integration step which is chosen for the flow field model.

$$\frac{\partial \rho_G Y_i}{\partial t} + \nabla(\rho_G v_G) = \bar{\omega}_m \quad (8)$$

Because of the coupling between pressure field and velocity field, the gas phase requires simultaneous solution of the mass and momentum equations to satisfy both balances. An approach based on the well-known SIMPLER algorithm [21] is applied to solve the momentum Eq. (9) in the porous bed. For the pressure field the ideal gas law is assumed. The pressure loss is estimated by Darcy’s law, based on the phase averaged velocity.

$$\frac{\partial}{\partial t}(\rho_G v_G) + \nabla(\rho_G v_G v_G) = -\nabla p - \frac{\mu}{K} v_G \quad (9)$$

Due to the dominance of convective transport, conduction within the gas phase is neglected in the energy Eq. (10). Source terms occur because of the convective heat and mass transfer between the solid and the gas phase and chemical reactions within the voids.

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_G c_v T) + \nabla(\rho_G v_G c_v T) \\ = -\nabla p v_G + \bar{\omega}_{con} + \bar{\omega}_{ch} + \bar{\omega}_{th} \end{aligned} \quad (10)$$

The source term due to convection between the solid phase and the gas phase is calculated as the sum total of convection terms over all  $n$  particles in a cell  $i$  Eq. (11), where the transfer coefficients are computed as stated above.

$$\bar{\omega}_{con} = \sum_{k=1}^n \alpha_k A_k \frac{1}{\Delta t} \int_0^{\Delta t} (T_{G,k} - T_{G,i}) dt \quad (11)$$

The sensible heat which is transported with the mass of  $m$  species between  $n$  solid particles in a volume element and the surrounding gas phase is calculated according to Eq. (12)

$$\bar{\omega}_{th} = \sum_{k=1}^n \sum_{j=1}^m \frac{1}{\Delta t} \int (c_v \dot{m}_{j,k} T_{S,k}) dt \quad (12)$$

Moreover, heat transfer due to conduction and radiation between the different particles occurs within a packed bed. This interaction has to be accounted for as a source term in the particle model. An approach to treat conduction by an

effective thermal conductivity is excluded, because the packed bed is not assumed as a homogeneous porous body. In the current application the bed process is resolved by single particle processes, which requires keeping track of particle cell and particle–particle relations. It is required to predict interaction between the solid and the gas phases and the solid particles, respectively. As wood contains only a small amount of ash, the solid will be fully depleted without any remaining residue. A particle diameter of 0.5 mm is chosen to be the minimum particle diameter appearing in the bed. If a particle reaches the minimum diameter it is removed from the computation.

The connectivity between neighbour particles in a bed allows the heat flux due to conduction between two particles to be calculated in the following form Eq. (13).

$$\dot{q}_{12} = - \frac{1}{\frac{1}{\lambda_1} + \frac{1}{\lambda_2}} \frac{\partial T}{\partial r} = - \frac{1}{\frac{1}{\lambda_1} + \frac{1}{\lambda_2}} \frac{T_{N1} - T_{N2}}{\Delta r_{N1} - \Delta r_{N2}} \quad (13)$$

The temperature gradient between two particles is approximated by the temperature difference between the outer shell values of the particles and the distance of the discretization points as indicated in Fig. 1b. As shown in Fig. 1c the contact area is assumed quadratic, which is determined by the contact angle  $\gamma$ . Hence, the contact area is given by

$$A_c = \frac{1}{2} ((R_1 \tan \gamma)^2 + (R_2 \tan \gamma)^2) \quad (14)$$

However, for solid fuels with low thermal conductivity, such as wood, conduction between solid particles only contributes to a small extent to the heat transfer in a packed bed.

Heat transfer due to radiation between the solid particles is a complex interaction of absorption, reflection and emission. Each particle emits a certain amount of heat to its surroundings depending on its surface temperature, area and emission coefficient. The radiative heat loss of each

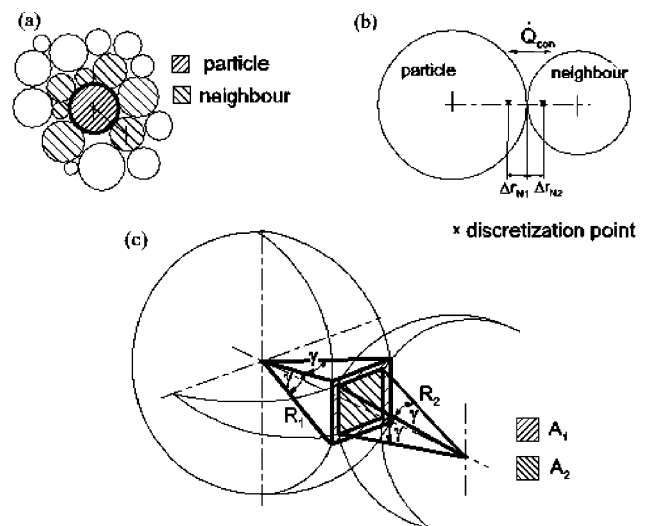


Fig. 1. Modelling of heat conduction in a packed bed of solid particles.

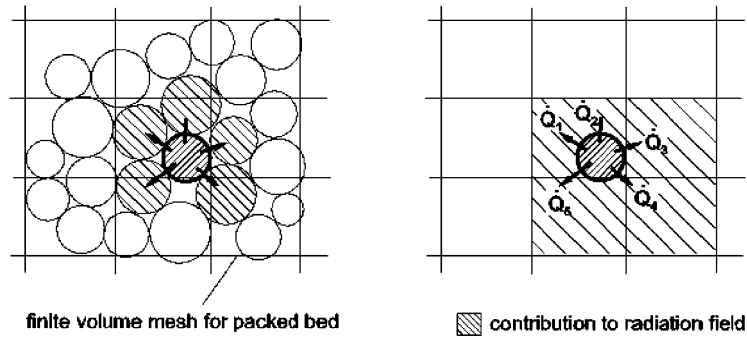


Fig. 2. Modelling of radiation in a packed bed of solid particles.

particle is distributed between  $n$  neighbour particles according to the surface area weighted ratio,

$$F_{i \rightarrow j} = \frac{A_i}{\sum_{j=1}^n A_j} \quad (15)$$

In order to account for reflection and transfer to particles not in direct contact with the emitting particle, the emanating radiation contributes to a radiation field related to the mesh of the flow field model, as shown in Fig. 2. The radiation terms of all particles in the bed result in a global radiation field to which the particles are exposed.

The radiation field also accounts for radiative heat transfer between the bed surface and the surroundings. Due to short ray travelling distances in the voids of the packed bed, adsorption, emission and scattering of the gas phase is neglected.

### 3. Results and discussion

To study conversion of a single wood particle, a test reactor was built up, Fig. 3. The cylindrical reactor, with an inner diameter of 50 mm, consists of a heated (reaction) zone (1) and a cooled part (2), where the particle rests until the reactor is heated to the desired temperature. When the temperature is reached, the particle is exposed to the reaction zone. The reactor temperature was kept constant during an experiment. To prevent oxygen from penetrating into the reactor during pyrolysis experiments, a nitrogen flow through the reactor is established (3). In char combustion, pure air was used as the carrier gas through the reactor. The particle is attached to a sample holder suspended from a precision balance (4). For each experiment, the mass loss of the particle and the evolution of the main gas species are recorded. Beech wood spheres of different diameters, with initial moisture content of 0, 30 and 67%, were used. Experiments were performed at various temperatures, diameters and moisture contents [22]. The mixture of carrier gas and production gas is extracted from the bottom of the reactor through a gas cleaning section (5) to prevent tar from entering the measuring devices.

Fig. 4 shows comparisons of experimental and predicted results for pyrolysis and char combustion of a single particle. Mass loss during pyrolysis was calculated by a simple single step pyrolysis model. The property data and kinetic data can be taken from Table 1. As the temperature during experiments is quite low while the oxygen content in the surrounding gas phase is high, only char conversion due to reaction with oxygen is taken into account in the model. The temperature does not reach a sufficiently high value for gasification reactions with water vapour of carbon dioxide to start. Kinetic data on char combustion with oxygen are given as intrinsic rate and can also be taken from Table 1.

Mass loss curves during pyrolysis are shown in Fig. 4a for different diameters of the dry beech wood particles at a reaction temperature of  $T_h = 743$  K. With increasing diameter of the particles, the mass loss rate decreases slightly. This indicates that, under the given conditions, the progression of pyrolysis depends on propagation of the heating front into the solid. The dependence on internal thermal resistance is captured well by the one-dimensional

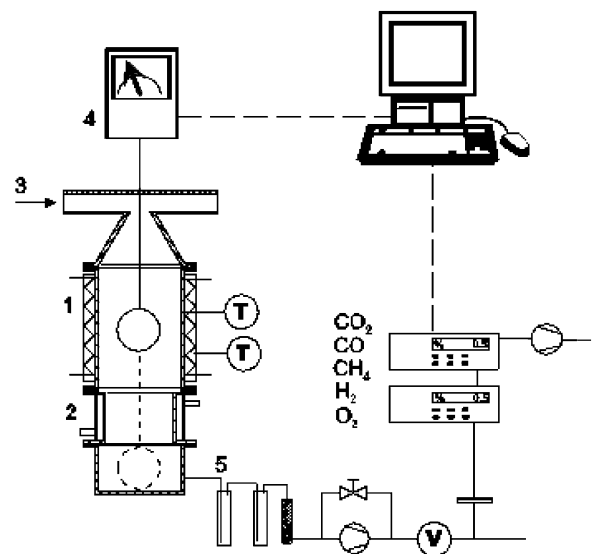


Fig. 3. Laboratory reactor for the conversion of a single fuel particle (1-heating, 2-cooling chamber, 3-carrier gas, 4-precision balance, 5-gas cleaning section).

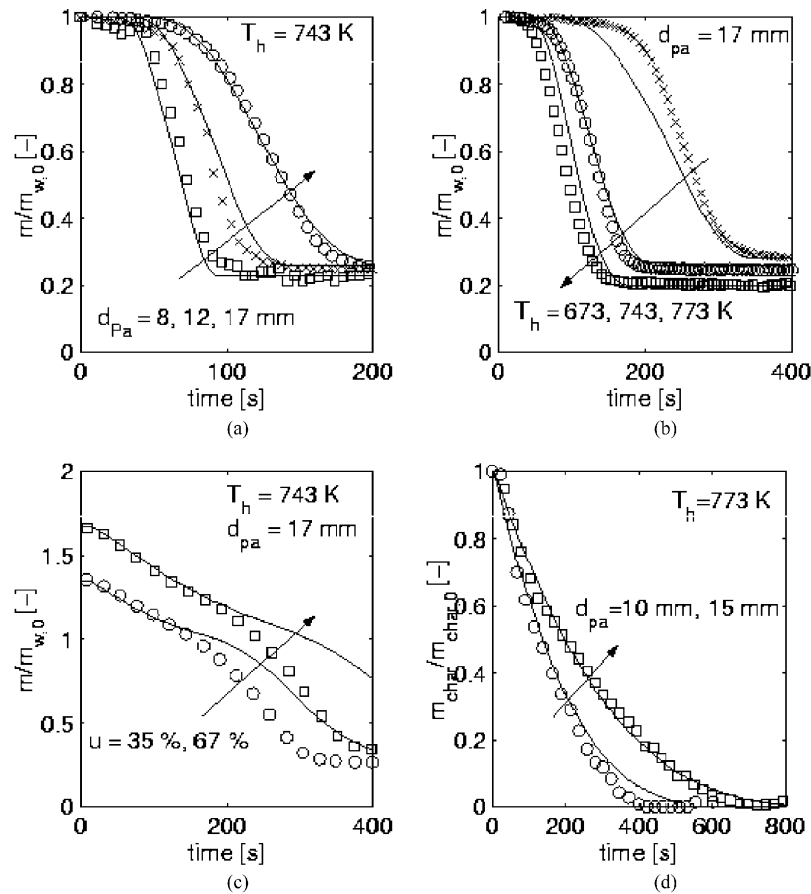


Fig. 4. Comparison of theoretical (solid lines) and experimental (symbols) data for a spherical beech wood particle in case of pyrolysis of dry wood (a,b), pyrolysis of wet wood (c) and combustion of wood char in air (d).

approach. Thus, the calculated values match the experimental results with sufficient accuracy.

For different reactor temperatures at a constant particle diameter of  $d_{pa} = 17$  mm, comparisons between experimental data and calculated values are shown in Fig. 4b. The theoretical values are in good agreement with the experimental data at reactor temperatures of  $T_h = 743$  and  $T_h = 773$  K. At  $T_h = 673$  K, calculations show an earlier start of pyrolysis than in the experiments. The difference between the experimental and the calculated values can be attributed to the drop in reactor temperature when the (cold) particle was transferred into the reaction zone. At higher temperatures, this drop was balanced out faster by the energy stored in reactor material.

Even if a simple pyrolysis model is used, the agreement between theoretical and experimental data is satisfying. Thus, applying kinetic data derived at dust samples to larger particles seems to be feasible by including description of the heat transfer. For property and kinetic data taken from literature no adaptation was necessary to match the results of dry wood particles.

Pyrolysis of wet wood particles with 33 and 67% water content, respectively, and a particle diameter of  $d_{pa} = 17$  mm at a reactor temperature  $T_h = 743$  K is

shown in Fig. 4c. The drying period of the wet wood is described well by the model based on a constant evaporation temperature, resulting in a steep drying front moving into the particle at a face velocity of roughly  $2.0 \times 10^{-5}$  and  $3.5 \times 10^{-5}$  m/s at a water content of 67 and 33%. Comparison with a drying model based on a heterogeneous reaction with pseudokinetic data taken from Ref. [17], showed an overestimation of the drying time and an overlapping with the pyrolysis process, which cannot be seen from the experiments. Assuming a constant evaporation temperature, drying and pyrolysis take place consecutively for the given particle diameters. However, for both water contents, the rate of pyrolysis is underestimated,

Table 1  
Property and kinetic data for wood and wood char used in calculation runs

	Beech wood	Wood char
$c_p$ (W/m <sup>2</sup> K)	$1500 + T$ [12]	$420.0 + 2.09T + 6.85 \times 10^{-4}T^2$ [12]
$\lambda$ (W/m K)	0.35 [12]	0.1046 [12]
$\langle \rho \rangle$ (kg/m <sup>3</sup> )	750 [24]	200 [23]
$k_0$ (1/s), (m/s)	$1.35 \times 10^9$ [25]	$3.01 \times 10^2$ [26]
$E_a$ (kJ/mol)	123.1 [25]	149.38 [26]
$A_i$ (m <sup>2</sup> /kg)	–	$2.71 \times 10^5$ [27]

Intrinsic rate.

indicating that the calculated temperatures at the end of the drying period are too low compared to the experimental values. Even though agreement between experimental and theoretical data is satisfying for pyrolysis of dry wood, the same property and kinetic data cannot be applied to wet wood. This may be explained by fractures and fissures within the solid which appear as a result of rapid evaporation during the drying period. In case of the experiments with dry wood samples, the virgin wood was dried at 120 °C for 24 h. The lower heating rate compared to the pyrolysis of wet wood does not enhance changes in the solid matrix. Thus, pyrolysis cannot be treated separately from the drying process before. The difference between experimental and theoretical mass loss histories increases with increasing water content. The change in the solid matrix will be influenced by several parameters, such as particle size, water content and temperature. This indicates that within a packed-bed model, which should be applied to thermal conversion of wet biomass, a possibility to consider this influence is required. Due to the varying boundary conditions each particle may experience in a packed bed, separate treatment of each fuel particle as realised in the given model allows to take these parameters into account. However, further experimental investigation is needed to

derive a relationship between water content, temperature, particle size and changes in the solid matrix.

For char combustion at  $T_h = 773$  K in pure air, mass loss curves for two different diameters of the particles are presented in Fig. 4d. In the computation runs, char is assumed to consist of pure carbon. The char was generated by pyrolysis of the beech wood particles. Even at a relatively low temperature, char combustion is completely boundary layer controlled, indicating the high reactivity which is typical of wood char. Under these conditions, char conversion can be described correctly by a shrinking-core model, resulting in a linear decrease of the particle radius with conversion, which was observed also for the calculations with the one-dimensional model. Agreement between the calculated and the experimental data is very good, showing that the mass transfer coefficient and reaction rate are described sufficiently accurate. Due to the boundary layer control of the process, the uncertainty of the kinetic data has no influence on the conversion of the solid. For char particles derived with wood at different water contents of the virgin material, no major difference in mass loss rates was observed during the experiments for the same particle diameter and reactor temperature as consequence of the boundary layer control of the process. Thus, for modelling

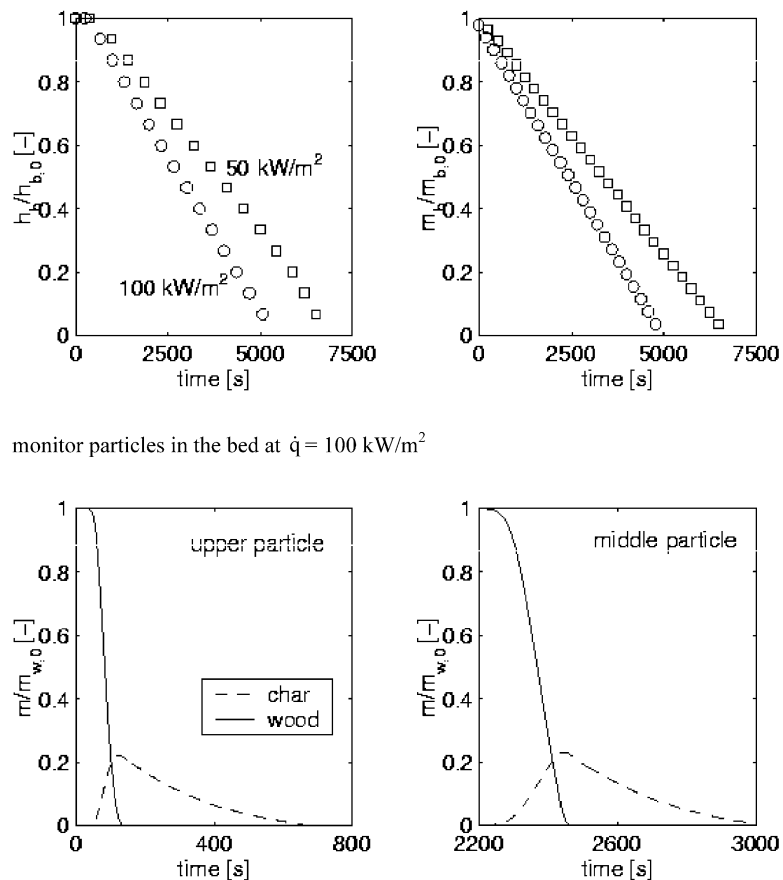


Fig. 5. Bed mass and height versus conversion time and mass loss history of monitor particles for a bed of beech wood particles with a heat flux of  $\dot{q} = 50$  and  $\dot{q} = 100$  kW/m<sup>2</sup> introduced from the top.

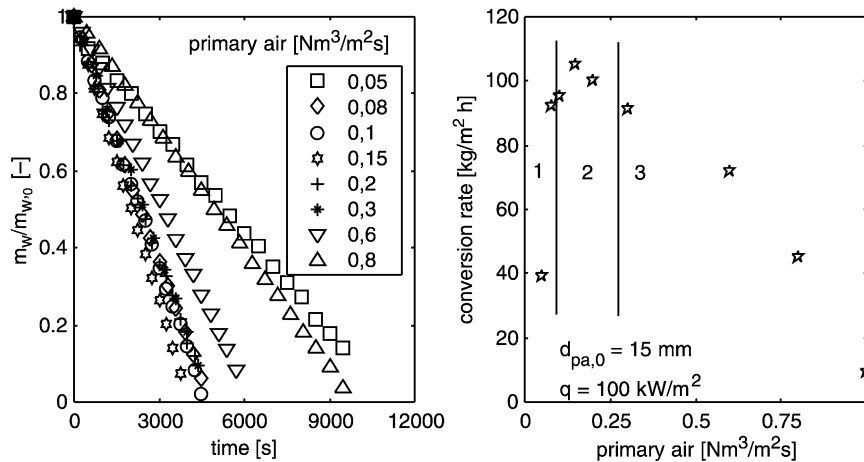


Fig. 6. Bed mass versus conversion time and average conversion rate versus primary air flow for a bed of beech wood particles exposed to a heat flux of  $\dot{q} = 100 \text{ kW}/\text{m}^2$ .

conversion of a packed bed of char particles with air under the given conditions the heat and mass transfer within each solid particle need not to be described separately allowing the application of simpler models such as given by Ref. [1]. However, in a model which can be applied to the whole conversion process of biomass, transport processes within the particles cannot be neglected.

With the same property data and kinetic data as for the single-particle problem discussed above, results for a one-dimensional pile of beech wood particles are shown in Fig. 5. The bed height is chosen to be 30 cm, and the initial particle diameter is  $d_{pa} = 15 \text{ mm}$  for all particles. Primary air at an inlet velocity of 0.2 m/s is supplied at the bottom, and a radiative heat flux of 50 and 100  $\text{kW}/\text{m}^2$ , respectively, is applied to the top of the bed. Fig. 5 shows height and mass of the bed versus the conversion time and mass loss histories for two particles in the bed at a heat flux of 100  $\text{kW}/\text{m}^2$ . The two particles are located in the upper cell and the middle cell of the bed mesh to monitor progression of the reaction front.

Bed mass decreases linearly with time, resulting in a grate combustion rate of 75  $\text{kg}/\text{h m}^2$  and 95  $\text{kg}/\text{h m}^2$  for a heat flux of 50 and 100  $\text{kW}/\text{m}^2$ , respectively. Even if only kinetic data derived from dust samples is used in the calculation, the values correspond to experimental results given by Ref. [6] for the combustion of wood particles on a grate. Due to the linear decrease of mass the overall conversion times of particles at different locations within the bed is comparable. This can also be seen from the mass loss histories of wood and char of the two monitor particles. The particle initially located at the top of the bed is pyrolysed immediately, due to the high heat flux in the upper part of the bed. Depletion of the char material starts after the particle has been fully pyrolysed. Thus no overlapping of the processes can be observed for these parameters. Limitation of the process by boundary layer diffusion causes the major part of the overall conversion time to be consumed by char combustion. Because of the lower heating rate the particle located at half of the bed

height has a pyrolysis period roughly twice as long as for the upper particle. Char conversion does not start until bed height is reduced to half of its initial value, when the particle is fully exposed to the heat flux from above, leading to a char conversion rate comparable to the particle originally located at the top of the bed Fig. 6.

For the parameters selected, combustion takes place mainly in the upper section and the temperature in the lower layers of the bed does not reach a sufficiently high level for char combustion to start. This results in a linear decrease of bed height with time which is qualitatively in good agreement with experimental results of Ref. [9].

#### 4. Conclusions

A numerical approach to predict the thermal conversion of a packed bed of wood has been presented. Within the method, the packed bed consists of a finite number of particles, whose individual processes are resolved by a particle model, applicable to each particle of a packed bed. It comprises heating, drying, pyrolysis, gasification and combustion on a one-dimensional and transient basis in conjunction with the relevant reactions.

However, the approach allows the need for macrokinetic data to be reduced and provides a deeper insight into the processes within a packed bed during combustion of a solid fuel. Comparisons show good agreement between experimental and theoretical results for the single particle model, indicating that the one-dimensional approach captures the main rate determining characteristics. Pyrolysis of wet particles at high heating rates requires further investigation into the structural changes of the solid matrix.

The particle processes are coupled to the gas flow in the voids of a packed bed through heat and mass transfer. The latter is described by a model to predict the flow of combustion gas in the void space of a packed bed by solving the conservation equations for mass, momentum and

energy. Even if no empirical correlation or specific data for a packed bed such as an effective thermal conductivity in the bed is used, agreement of the results with values of experimental studies from the literature is satisfactory. Thus, the approach of the model to divide the packed bed into its particles seems feasible, to capture the main rate limiting parameters, allowing to take particle diameters and properties into account. However, further research is required to validate, e.g. the description of the heat transfer within the bed.

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## References

- [1] Ford N, Cooke M, Sage P. Modelling of fixed bed combustion. *Fuel Process Technol* 1993;36:55–63.
- [2] Fatehi M, Kaviany M. Adiabatic reverse combustion in a packed bed. *Combust Flame* 1994;99:1–17.
- [3] Raupenstrauch H. Ein Beitrag zur Computersimulation reagierender Schüttschichten. PhD Thesis. Technical University Graz; 1990.
- [4] Hartner P. Entwicklung eines Computerprogramms zur eindimensionalen Simulation von heterogenen Festbett- und Vorschubreaktoren. PhD Thesis. Technical University Graz; 1996.
- [5] Beckmann M, Scholz R. Simplified mathematical model of combustion in stoker systems. *Third Eur Conf Ind Furnaces Boilers* 1995;18/21:61–70.
- [6] Kuo JT. Estimation of burning rates in solid waste combustion furnaces. *Combust, Sci Technol* 1998;137:1–29.
- [7] Goh YR, Siddal RG, Nasserzadeh V, Zakaria R, Swithenbank J, Lawrence D, Garrod N, Jones B. Mathematical modelling of the burning bed of a waste incinerator. *J Inst Energy* 1998;71:110–8.
- [8] Saastamoinen J, Haukka P. Simultaneous drying and pyrolysis in fixed bed combustion of wet biomass. *Proceedings of the 11th International Drying Symposium, Halkidiki*; 19–22 August 1998. p. 1975–1982.
- [9] Shin D, Choi S. The combustion of simulated waste particles in a fixed bed. *Combust Flame* 2000;121:167–80.
- [10] Maschio G, Lucchesi A, Koufopoulos C. Study of kinetic and transfer phenomena in the pyrolysis of biomass particles. *Adv Thermochem Biomass Conversion* 1994;.
- [11] Miller RS, Bellan J. Analysis of reaction products and conversion time in the pyrolysis of cellulose and wood particles. *Combust Sci Technol* 1996;119:331–73.
- [12] Grønli M. A theoretical and experimental study of the thermal conversion of biomass. PhD Thesis. NTNU, Trondheim; 1996.
- [13] Saastamoinen J, Impola R. Drying of biomass particles in fixed and moving beds. *Proceedings of the 10th International Drying Symposium, Krakow*; 30 July–2 August, 1996.
- [14] Gnielinski V. Berechnung des Wärme- und Stoffaustauschs in durchströmten ruhenden Schüttungen. *Verfahrenstechnik* 1982;16(1).
- [15] Schröder E. Bestimmung des Druckverlustes und des Wärmeüberganges von gasdurchströmten Feststoffschüttungen in der Pantha Anlage. Report 6373, Research Centre Karlsruhe; 1999.
- [16] Bruch C, Peters B, Nussbaumer T. Modellierung der Festbettverbrennung am Beispiel des Brennstoffes Holz. *German Flame Days, Dresden*; 14–15 September 1999. p. 139–44.
- [17] Chan WR, Kelbon M, Krieger BB. Modelling and experimental verification of physical and chemical processes during pyrolysis of a large biomass particle. *Fuel* 1985;64:1505–13.
- [18] Heidenreich C, Zhang D. Measuring the temperature response of large wet coal particles during heating. *Fuel* 1999;78:991–4.
- [19] Peters B, Bruch C. Evaluation of ODE-solvers for the prediction of thermal conversion of solid fuel particles. *16th IMACS World Congress, Lausanne*; 21–25 August 2000.
- [20] Peters B. A detailed model for devolatilization and combustion of waste material in packed beds. *Third European Conference on Industrial Furnaces and Boilers, Porto*; 1995. p. 86–104.
- [21] Patankar SV. *Numerical heat transfer and fluid flow*. New York: McGraw-Hill; 1980.
- [22] Schaeffer B, Wyrtsch F. Diploma Thesis. ETH Zurich, Department of Energy Technology; 2000.
- [23] Kansa EJ, Perlee HE, Chaiken RF. Mathematical model of wood pyrolysis including internal forced convection. *Combust Flame* 1977;29:311–24.
- [24] Petek J. Experimentelle Untersuchung der Pyrolyse in inerter und reaktiver Atmosphäre unter den Bedingungen der Wurfbeschickung. PhD Thesis. Technical University Graz; 1998.
- [25] Balci S, Dogu T, Yücel H. Pyrolysis kinetics of lignocellulosic materials. *Ind Engng Chem Res* 1993;32:2573–9.
- [26] Caram HS, Amundson NR. Diffusion and reaction in a stagnant boundary layer about a carbon particle. *Ind Engng Chem Fundam* 1977;16:171–81.
- [27] van den Aarsen FG, Beenackers A, van Swaaij W. Wood pyrolysis and carbon dioxide char gasification kinetics in a fluidized bed. *Fundam Thermo-chem Biomass Conversion* 1985; conversion.