Development of a streak formation model for an improved prediction of gas phase combustion in biomass grate furnaces

Ali Shiehnejadhesar1,2, Ramin Mehrabian2, Robert Scharler1,2,3, Ingwald Obernberger1,3

1 Graz University of Technology, Institute for Process and Particle Engineering, Inffeldgasse 21B, 8010 Graz, Austria; Tel: +43(0)3168739230; Fax: +43(0)3168739202; Email: Ali.shiehnejad@bioenergy2020.eu
2 BIOENERGY 2020+ GmbH, Inffeldgasse 21B, 8010 Graz, Austria
3 BIOS BIOENERGIESYSTEME GmbH, Inffeldgasse 21B, 8010 Graz, Austria

Abstract

State-of-the-art packed bed models supply continuous concentration profiles as boundary conditions for subsequent CFD simulations of gas phase, leading to pre-mixed combustion conditions. However, in reality the “porous” nature of the packed bed leads to streak formation influencing gas mixing and combustion. Therefore, in the present work, in order to account for the influence of the streaks on gas phase combustion, a gas streak model based on a correlation between the local gas residence time and a mixing time has been developed based on numerical simulations and tested for a real-scale grate furnace. The streak model is based on the mixing function to describe the mixing process above the fuel bed. The mixing function is a combination of the mixing time, the necessary residence time to reach the fully mixed condition, and the flue gas residence time in the region above the fuel bed.

A CFD case study with an ideally packed bed with spheres as fuel particles and non-reacting flow was performed to numerically derive the mixing time. The particle diameter was derived from the volume to surface area ratio of pellets according to Austrian standard. The volatiles were represented by CO2 released from the surface of the particles. The volatiles release rate from a single particle was approximated by the value of an in-house developed model for single particle conversion. The influence of relevant parameters, like bed height, volatiles mass flow rate and particle Reynolds number (calculated with the bulk flow velocity of primary air below the bed and the particle diameter), on mixing time was investigated.

The results showed a strong influence of the number of layers (bed height) on mixing. Hence, it was considered as independent parameter. As a next step, three different heights with different numbers of particle layers (5, 10 and 15 layers) were chosen to investigate the influence of particle Reynolds number and volatiles release rates. The results show a negligible effect of the volatiles release rate on mixing. However, the particle Reynolds number has a significant effect on the mixing time. For all layers considered, a trend concerning the mixing time in dependence of the particle Reynolds number was found. The results of this study serve as look-up table for the calculation of the mixing time in dependence of the different influencing parameters.

Finally, the model was linked with an in-house developed hybrid gas phase combustion model suitable for low as well as highly turbulent combustion conditions and tested for a 180 kWth pilot-scale grate furnace. The results in comparison with a simulation without the streak formation model show, that the temperature and flue gas species prediction can be improved with the proposed streak formation model. Especially, in the region above the fuel bed (in the primary combustion chamber), this is of special importance for NOx reduction by primary measures.

Keywords

CFD modelling, biomass, combustion, grates furnace, streak formation model, hybrid model
1. Introduction and objectives

CFD modelling is becoming increasingly important for the development and optimisation of biomass grate furnaces. Here, gas phase combustion models play a key role concerning predictions of flow, temperature, and gaseous emissions (e.g. CO and NOx).

The mode of gas combustion in a grate furnace can be classified as partially premixed with a locally different mixing degree of oxidiser and fuel, whereas in this context the combustible gases released from the solid biomass fuel bed are to be understood as (gaseous) fuel.

An empirical packed-bed model developed by TU Graz in cooperation with BIOS [1] is usually being used at BIOENERGY 2020+ for the calculation of composition, temperature and flue gas leaving the surface of the solid biomass fuel bed. The empirical packed-bed model, as most of the common packed bed models, calculates profiles of partially premixed flue gas compositions not considering spatial concentration gradients of oxygen and volatiles since the fuel particles and the surrounding space cannot be resolved. However, in reality, the amount and distribution of combustibles and oxidiser in the gas released from the biomass particles in the fuel bed are locally strongly differing. Therefore, the “porous” nature of the packed bed leads to streak formation influencing gas mixing and combustion, which is not described by state-of-the-art CFD-based packed bed models.

Therefore, in this paper a model which accounts for the influence of the streaks on gas phase mixing and reactions (combustion, NOx formation) is introduced. The streak model is based on a correlation between the local gas residence time and mixing time, whereas the mixing time is defined as the necessary residence time to reach the fully mixed condition. The mixing time was derived based on a series of numerical simulations with an ideally packed bed with spheres representing the biomass particles.

Finally, the streak model was linked with an in-housed developed hybrid gas phase combustion model suitable for laminar to highly turbulent combustion conditions and applied for a pilot-scale grate furnace (180 kWth) of BE2020+ concerning the simulation of gas phase combustion and NOx formation. For the purpose of model evaluation, the simulation results were compared with CO and NOx emission measurements and simulations without the application of the streak formation model.

2. Methodology

The paper is structured as following: Firstly, an overview of the models applied for the case studies is given in the modelling part. Then, the non-reacting packed bed simulations to derive the streak formation parameters are described. Finally, the case study (pilot-scale grate furnace of BE2020+) for the application of the streak formation model is introduced.

2.1 Modelling

In this chapter, all the models used for the non-reacting packed bed simulations as well as the grate furnace simulations are explained. Then, the hybrid gas phase combustion model which is utilised for the grate furnace simulations is introduced. Finally, the streak formation model is presented.

2.1.1 Model overview

For the derivation of streak formation parameters, non-reacting multi-species simulations with an ideally packed bed with spheres have been performed. The SST k-ω low Reynolds turbulence model is applied to cover the whole range of flow conditions from laminar to turbulent flows in biomass grate furnaces. The primary air is injected uniformly below the fuel particles whereas the grate has been neglected. CO2 is taken as trace species representing the volatiles release through the particle surface. To estimate the degree of mixing, a mixing state is defined (see section 2.1.3). The mixing time is evaluated based on an estimated residence time to achieve a certain degree of mixing. The gas residence time is calculated by solving a scalar transport equation.

For the simulation of the pilot-scale grate furnace of BE2020+, the following models have been applied: an empirical model developed by TU Graz in cooperation with BIOS [1] is used to describe the thermal decomposition of the solid biomass fuel. The model consists mainly of three parts. The
definition of one-dimensional profiles along the grate concerning the degradation of the fuel components as well as fuel drying (part 1 based on assumptions and experimental data forms the basis). In combination with the definition of conversion parameters (based on assumptions as well as experimental and literature data), which describe the formation of the most important flue gas components \( \text{CH}_4, \text{CO}, \text{CO}_2, \text{H}_2, \text{H}_2\text{O}, \text{O}_2 \) as well as \( \text{NH}_3, \text{HCN} \) and \( \text{NO} \) (part 2), the stepwise balancing of mass and energy fluxes released from the fuel bed is possible (part 3) [1, 2, and 3]. The calculation results are used as boundary profiles for subsequent CFD simulations of the turbulent reactive flow in the furnace. For modelling of the turbulent reactive flow in the combustion chamber the Realizable \( k-\varepsilon \) model (turbulence), the Discrete Ordinates Model (radiation) as well as the Hybrid model (gas phase combustion) have been applied. Together with the Realizable \( k-\varepsilon \) model, the enhanced wall treatment model is used, which covers a two-layer turbulence approach combined with enhanced wall functions [4]. The model is valid throughout the near-wall region (i.e., laminar sub-layer, buffer region, and fully-turbulent outer region). Therefore, the model is supposed to be valid for low and high Reynolds wall-bounded flows.

Under the assumption that \( \text{NO}_x \) formation reactions do not significantly influence the flow pattern in the furnace, a time saving 2-step approach is applied for CFD simulations. The basic gas phase combustion simulation has been performed using the hybrid combustion model (two simulations without and with the effect of streaks) with a C-H-O subset of the Skeletal Klippen97 mechanism (12 species and 25 reactions) [5], which has extensively been validated for grate furnaces [6]. The subsequent CFD simulation of gas phase fuel \( \text{NO}_x \) formation in a post-processing mode has been done using the hybrid model in combination with a detailed reaction mechanism (28 species and 102 reactions in total) [6].

2.1.2 Hybrid gas phase reaction model

An in-house developed hybrid gas phase reaction model suitable for laminar to highly turbulent flows has been applied for the simulation of the reacting gas flow. In particular, in the region above the fuel bed and in small-scale biomass combustion plants, gas phase mixing is highly influenced by laminar and low turbulence zones. Here, the Eddy Break-Up combustion models are not valid because they were originally developed for highly turbulent flows. Therefore, a hybrid Eddy Dissipation Concept (EDC) / Finite Rate Kinetics model (FRK) has been developed, which calculates the effective reaction rate from laminar finite rate kinetics and the turbulent reaction rate and weights them depending on the local turbulent Reynolds number of the flow.

For a multi-component system, the species mass conservation equation is defined as follows;

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i) = -\nabla \cdot \mathbf{J}_i + R_i \quad (1)
\]

Where \( \rho \) is the mixture density, \( Y_i \) is the mass fraction of species \( i \), \( \mathbf{u} \) is the velocity vector, \( \mathbf{J}_i \) is the diffusion flux of species \( i \) due to concentration gradients, and \( R_i \) is the net rate of production of species \( i \) by chemical reactions.

In the hybrid model, the mean chemical reaction (second term in the right hand side of Eq. (1)) is modelled as:

\[
(R_i)_{\text{Hybrid}} = \left( \frac{1}{1 + \text{Re}_t} \right) (R_i)_{\text{FRK}} + \left( \frac{\text{Re}_t}{1 + \text{Re}_t} \right) (R_i)_{\text{EDC}} \quad (2)
\]

where \((R_i)_{\text{FRK}}\) is the FRK mean reaction rate, the term \((R_i)_{\text{EDC}}\) is the mean reaction rate calculated by the EDC model and \( \text{Re}_t \) is the turbulent Reynolds number \(( \text{Re}_t = \frac{\rho \mathbf{u}^2}{\nu \varepsilon} )\). The hybrid model has been extensively validated for a series of diffusion jet flames covering laminar, transitional, and turbulent flow conditions. A detail description of the hybrid gas phase reaction model can be found in [7].
2.1.3 Streak formation model
A streak formation model has been developed. The model is based on a mixing time, where the gas streaks arising from the fuel bed are fully mixed, and a correlation with the residence time of the flue gas released from the fuel bed. In order to describe the mixing process above the packed bed, a criterion has been defined to calculate the mixing state (MS) as following:

\[
MS = \left(1 - \frac{C_{fm} - C(t)}{C_{fm}}\right)
\]

Here, \(C_{fm}\) is the tracer gas concentration (here CO\(_2\)) in the fully mixed gas and \(C(t)\) is the local tracer gas (CO\(_2\)) concentration in dependence of the mixing time. The residence time which is necessary to reach the defined mixing state (here, 0.99 < MS < 1.01 has been defined) is the mixing time \(t_{fm}\).

Finally, the mixing function (MF) is the combination of the mixing time \(t_{fm}\) and the gas residence time \(t_{gas}\):

\[
MF = \min\left(\frac{t_{gas}}{t_{fm}}, 1\right)
\]

where

MF = 0 (completely unmixed)
MF = 1 (completely mixed)

A scalar transport equation has been solved to calculate the gas residence time as following [8]:

\[
\frac{\partial}{\partial x_i} \rho u_i \varphi - J \frac{\partial \varphi}{\partial x_i} = \rho \left(\bar{J} = -\rho(D_m + D_t) \frac{\partial \varphi}{\partial x_i}\right)
\]

Here, \(\rho\) and \(u_i\) are density and velocity of the flue gas; \(\bar{J}\) is a component of diffusion flux; \(D_m\) and \(D_t\) are molecular and turbulent diffusivity. \(\mu_t\) is the turbulent viscosity and \(Sc_t\) is the turbulent Schmidt number (with a value of 0.7 which is also applied for the species transport equation).

After the flow field is solved with CFD simulations, the values of residence time are approximated by solving Eq. (5). The first and second terms on the left hand side of Eq. (5) represent the convection and diffusion fluxes, the density on the right hand side represents the source term. The later means, that the residence time in each computing cell will be added to the residence time calculated by the transport equation. Eq. (5) has been implemented by a user-defined function (UDF) in ANSYS FLUENT.

As a first approximation, a linear correlation between the gas residence time \(t_{gas}\) and the mixing function MF has been chosen. A CFD-based case study with an ideally packed bed has been defined in order to numerically derive the mixing time \((t_{fm})\). Finally, the effective reaction rate is calculated by multiplying the mixing function, which defines the macro-mixing state, with the reaction rate, calculated by the hybrid combustion model as following:

\[
(R_i)_{\text{Hybrid-streak formation}} = MF \times (R_i)_{\text{Hybrid}}
\]

2.2 Case study for the derivation of the streak formation model constants
A CFD-based case study with an ideally packed bed with spheres as fuel particles and non-reacting flow has been performed in order to numerically derive the mixing time. The volatiles were represented by CO\(_2\) released from the surface of the particles in the bed. The volatiles release rate from single particles was approximated by an in-house developed layer model [9] for the conversion of thermally
In this parameter study, the following influencing parameters have been investigated for a packed bed:

- Bed heights: variation by particle layers (from 5 to 15 layers)
- Volatiles mass flow rate: During typical biomass combustion conditions with air staging the most relevant components released are H₂O, CO₂, CO, H₂ and CH₄ [10, 11 and 12]. However, during packed bed combustion, the dominant gas volume flux is from the primary air passing through the packed bed. In CFD simulations the density of the mixture is usually considered as incompressible (due to the low pressure changes) and mainly depends on the temperature inside the combustion chamber that influences the volume flow rate of the volatiles released from the biomass particles. Moreover, since a non-reacting simulation is performed, for the release rates only an average value can be estimated. Therefore, a sensitivity analysis concerning the influence of the volatiles release rate was performed. In order to cover the possible range of released volume fluxes, the estimated value of the reference case was multiplied by a factor x. A typical volatiles release rate was estimated with the layer model; for the investigation of the sensitivity of the results on the release rates, this value has been varied between a factor from 1 to 1.7. It could be shown that the influence of the release rate is comparably low.

- Bulk flow velocity of primary air below the bed (0.1 - 7 m/s): In biomass grate furnaces, the flow above the fuel bed is typically in the low Re range. Which primary air velocities varying from 0.1 to 3 (m/s). The values are gained from an in-house developed empirical packed bed model of TU Graz and BIOS. Therefore, to cover all ranges of flow conditions for small to large-scale biomass combustion plants, the sensitivity analysis has been performed.

The diameter of the spheres was approximated based on the volume to surface area ratio of pellets according to the respective EU standard. As mentioned, the study has been performed for pellets as fuel. However, the simulation results can be applied for all particle sizes by applying the particle Reynolds number for the look-up table where the results are summarised. Here, three parameter studies with an ideally packed bed were performed in order to calculate the mixing time in dependence of the influencing parameters. Figure 1 shows the CFD domain of the packed bed for 5 layers considered in this study. The primary air was injected below the bed with an even distribution and the volatiles represented by CO₂ as tracer gas were released from the surface of the spheres. Moreover, different planes above the bed were defined to evaluate the mixing state and mixing time. A simulation matrix was built for each layer to derive the mixing time based on the primary air velocity and volatiles mass flow rate. The flow simulation was performed for all primary air velocities and volatile mass flow rates. Then, the mixing state was calculated at each plane defined above the bed. Finally, the mixing time was derived based on the estimated gas residence time which is necessary to reach the defined mixing state (here, 0.99 < MS < 1.01).

Figure 1: CFD domain and boundary conditions for the evaluation of the mixing time above the packed bed
Therefore, the mixing time can be represented by influencing parameters like primary air velocity and number of layers considered in the simulations. To make the model applicable for all fuel particle sizes, the mixing time can be represented as function of the particle Reynolds number instead of primary air velocity. The particle Reynolds number can be defined as particle diameter times primary air velocity divided by the kinematic viscosity of air \( \text{Re}_p = \frac{V_{\text{primary air}} d_p}{\nu_{\text{air}}} \). The volume diameter \( d_v \) [13] can be derived based on the diameter of a sphere having the same volume as the biomass particles. The biomass particle volume can be estimated from the average size of the biomass particles.

2.3 Test and verification of the streak formation model

To investigate and verify the influence of the streak formation model on gas phase mixing and reactions, a CFD simulation was performed for a pilot-scale moving grate furnace equipped with a hot water fire tube boiler (180 kW\(_{th}\)) using wood chips as fuel. Table 1 provides the most relevant operating conditions of the furnace and the fuel composition.

The pilot-scale moving grate furnace used for the test of the streak formation model is shown in Figure 2. The simulation domain comprises the combustion chamber above the fuel bed till the exit of the hot water fire tube boiler. Recirculated flue gas can be supplied below the grate and through six nozzles above the fuel bed. The furnace has been designed to switch between a short and a long primary combustion zone. The short primary combustion chamber is achieved by activating the first secondary nozzle row and closing the second secondary air nozzle row and vice versa for the long primary combustion zone.

In this case study the first secondary air nozzles (eight nozzles) were closed and secondary air was injected through six nozzles at the entrance to the third horizontal duct. Besides, there was no flue gas recirculation applied neither below the grate nor through the flue gas recirculation nozzles. False air leaking into the combustion chamber due to non-perfect sealing of the fuel feeding system was injected via the fuel supply. A certain amount of leakage air (10% of primary air), obtained from the measurements during the test run, was taken into account in the simulation as false air. Due to the symmetry of the furnace, only half of the furnace was simulated. Therefore, the symmetry boundary condition was used in the mid plane of the furnace.

![Figure 2: Geometry of the pilot-scale moving grate biomass furnace of BIOENERGY2020+ with a fire-tube hot water boiler](image-url)
The water side of the fire tube boiler walls was not included in the simulation. A convection boundary condition with 85°C (average water temperature) and a typical heat transfer coefficient for water in forced convection (6000 W/m²K) was used for the fire tube boiler walls.

Table 1: Operating conditions and fuel characteristics of the pilot-scale grate furnace

<table>
<thead>
<tr>
<th>Operating conditions</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal boiler load</td>
<td>kW</td>
<td>155</td>
</tr>
<tr>
<td>Adiabatic flame temperature</td>
<td>°C</td>
<td>1325</td>
</tr>
<tr>
<td>Flue gas recirculation ratio</td>
<td>-</td>
<td>0</td>
</tr>
<tr>
<td>(\lambda_{\text{Prim}})</td>
<td>-</td>
<td>0.52</td>
</tr>
<tr>
<td>(\lambda_{\text{Total}})</td>
<td>-</td>
<td>1.41</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fuel composition</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ash</td>
<td>Mass fraction d.b.</td>
<td>0.76</td>
</tr>
<tr>
<td>C</td>
<td>Mass fraction d.b.</td>
<td>49.70</td>
</tr>
<tr>
<td>H</td>
<td>Mass fraction d.b.</td>
<td>6.00</td>
</tr>
<tr>
<td>O</td>
<td>Mass fraction d.b.</td>
<td>43.50</td>
</tr>
<tr>
<td>N</td>
<td>Mass fraction d.b.</td>
<td>0.08</td>
</tr>
<tr>
<td>S</td>
<td>mg/kg d.b.</td>
<td>62.00</td>
</tr>
<tr>
<td>Moisture content</td>
<td>Mass fraction w.b.</td>
<td>41.90</td>
</tr>
<tr>
<td>GCV</td>
<td>MJ/kg d.b.</td>
<td>19.9</td>
</tr>
<tr>
<td>NCV</td>
<td>MJ/kg w.b.</td>
<td>9.8</td>
</tr>
</tbody>
</table>

Explanations: w.b.: wet basis; d.b.: dry basis; GCV: gross calorific value; NCV: net calorific value; \(\lambda_{\text{Prim}}\): primary air ratio related to primary air supplied below the grate; \(\lambda_{\text{Total}}\): total air ratio related to total amount of air supplied.

3. Discussion of results

3.1 Derivation of streak formation model constants

An initial case study showed a strong effect of the number of layers (bed height) on mixing (not shown here). Hence, it was considered as an independent parameter. Afterwards, a simulation matrix was defined in order to investigate the effect of primary air velocity and volatiles mass flow rate variations on the mixing (mixing state) for each number of particle layers defined (5, 10, and 15 layers). Moreover, to reduce the number of independent parameters (here, particle diameter and primary air velocity) from two to one, the particle Reynolds number was defined (see section 2.2).

The results showed a negligible effect of the volatiles release on mixing (not shown here). However, the primary air velocity and particle Reynolds number respectively, had a significant effect on mixing. Figure 3 shows the mixing time behaviour in dependence of the particle Reynolds number as well as the number of layers. For all layers considered, a trend concerning the mixing time in dependence of the particle Reynolds number was found. The results showed that the mixing time of the streaks increases as the particle Reynolds number increases. Generally, at lower particle Reynolds numbers the mixing time is lower. This attributes to a higher residence time of the flue gas due to lower primary air velocities that improve the mixing of primary air and volatile matter. The mixing time increases as the particle Reynolds number (i.e. primary air velocity) rises. Moreover, the mixing time at all particle Reynolds numbers is lower for a packed bed with larger height since a higher residence time inside the packed bed improves mixing of primary air and volatile matter. The results of this case study serve as look-up table for the calculation of the mixing time in dependence of the different influencing parameters. For practical application (e.g. the furnace simulation with the streak formation model - see section 3.2) the mixing time \((t_{\text{mix}})\) can be retrieved by a linear interpolation between the calculation points through an estimation of the particle Reynolds number and the number of layers. The particle Reynolds number can be easily calculated from the velocity profile specified by the empirical packed
bed model along the grate and the particle diameter (e.g. volume diameter [13]). Besides, the number of layers can be estimated by the initial estimated height of the packed bed and the diameter of the fresh biomass fuel fed. The number of layers represents the number of particles that can be stacked in that length (e.g. length divided by the diameter of particles). Since the total number of particles on the bed remains constant on an average, also the number of layers remains constant over the grate length.

![Figure 3: Mixing time [sec] for different particle Reynolds numbers and different numbers of particle layers](image)

**3.2 Test of the streak formation model for a biomass grate furnace**

In this section, the results for the simulation of the 180 kW biomass grate furnace of BIOENERGY 2020+ are shown. To see the effect of streaks on the gas reactions concerning temperature and species (e.g. CO and NOx formation), two simulations were performed, without and with the streak formation model. Figure 4 (left) shows the calculated particle Reynolds number as well as the number of layers along the grate. The particle Reynolds number was calculated based on the velocity profile calculated with the empirical packed bed model (the maximum primary air velocity is about 0.5 [m/s] in the present case). The particle diameter was estimated from the volume diameter (see section 2.2) (the wood chips particles were assumed as spheres with a \( d_v = 25 \) [mm]). Besides, the number of layers can be estimated by the initial estimated height of the packed bed and the diameter of the fresh wood chips fed. To derive a mixing time profile along the grate, (Figure 4 [right]) the values were retrieved from the look-up table for the mixing time (as described in section 3.1).

The shrinkage of particles was implicitly considered in the simulations by the assumption of the shape of the fuel bed and the assumption of a constant number of particle trajectories along the grate length. For example, the particle size changes as the particles move along the grate (i.e. the diameter of particles decreases). However, the number of particles remains constant during the conversion processes along the grate which is considered in the simulations. Hence, the particle size variation affecting the particle Reynolds number along the grate is considered in the simulations.

Finally, two transport equations were solved, one for the gas residence time and the other for the mixing time, to derive the local mixing function defined in Eq. 4. Figure 5 shows the contour plots of gas residence time (left) and the mixing function (right) derived from Eq. 4.
Figure 4: Particle Reynolds number [-] and number of particle layers [-] (left) as well as estimated mixing time [sec] interpolated from calculation points of Figure 3 (right).

Figure 5: Gas residence time [sec] (left), and mixing function [-] (right).

Figure 6 shows the flue gas temperature predicted with the hybrid model (left) and the hybrid-streak formation model (right). The calculated CO concentrations for both hybrid and hybrid-streak formation model are shown in Figure 7. As can be seen from both figures (temperature and CO concentrations), there are no big differences between the two models. This can be explained by a staged combustion with $\lambda_{PCZ} < 1$ and sufficient residence time in the primary combustion zone for a full consumption of $O_2$ and, hence a flue gas composition at the entrance to the secondary combustion zone, which is approximately independent from the combustion model. Furthermore, the reaction progress is not influenced by the streaks from the packed bed anymore and the residence time in the secondary combustion zone is high enough for an almost complete CO burnout. Therefore, the effect of streak formation on the combustion process (flue gas temperature and CO burnout) for this specific case is not distinctive. Moreover, in the present test case, the CO emission's measured at boiler outlet was very low. Therefore, in this specific case study, the influence of the models applied in the simulation (hybrid and hybrid-streak formation model) on CO emissions could not be validated. Therefore, further validation simulations are currently being performed for other cases. The predicted $O_2$ mass fraction calculated with both models is depicted in Figure 8. The oxygen concentration above the bed is predicted slightly different in both cases. The $O_2$ concentrations are influenced by the streaks above the fuel bed especially in the locations where they are highlighted (location 1 and 2). The
characteristics of reacting radicals (e.g. OH and O) are of high relevance for an in-depth understanding of the combustion and NO\textsubscript{x} formation processes \cite{14}. These radicals are of high relevance especially for the formation of NO\textsubscript{x}. The calculated OH and O species with hybrid and hybrid-streak formation models are shown in Figure 9. The OH and O species are generally lower predicted with the hybrid-streak formation model.

This is mainly due to the contribution of the streak formation model (i.e. the spatial distribution of oxygen concentrations (see Figure 8)) in which the rates of production or destruction of the species are slowed down by the streak formation model (see Eq. 6). Since the net reaction rate in the streak formation model is multiplied by the mixing function, the region above the major flue gas release zone and the adjacent shear layers / reaction fronts are mainly influenced by mixing of the streaks.

Figure 6: Flue gas temperature field calculated by the hybrid model [°C] (left) and the hybrid-streak formation model (right)

Figure 7: Iso-surfaces of CO concentration [ppmv] in the mid plane of the computational domain calculated by the hybrid model (left) and the hybrid-streak formation model (right)
Figure 8: Iso-surfaces of the $O_2$ mass fraction [-] in the mid plane of the computational domain calculated with the hybrid model (left) and the hybrid-streak formation model (right)

Figure 9: Iso-surfaces of $O$ concentration [ppmv] (left), and $OH$ concentration [ppmv] (right) calculated with the hybrid (top) and the hybrid-streak formation model (bottom)

As already mentioned, a skeletal reaction mechanism (28 species and 102 reactions in total) was applied [6] for the simulation of the NO$_x$ formation process, whereas the simulation was performed in a post-processing step. The initial conditions were taken from the previous solution data (combustion simulation with hybrid and hybrid-streak formation model, respectively).

Experimental data of the combustion and release behaviour for a variety of solid biomass fuels have been gained through several measurement campaigns in a lab-scale pot furnace reactor (packed bed batch reactor) [15, 16]. These experimental data include the concentration profiles of the N containing species NO, NH$_3$, HCN, NO$_2$ and N$_2$O over time. The measured profiles are utilised for the derivation
of release functions for the most relevant NOx precursors measured. The release functions of fuel nitrogen depend on the local air ratio (lambda) and the nitrogen content of the fuel. The most important NOx precursor detected above the fuel bed under fuel rich conditions is NH3, while HCN is almost insignificant. NO is detected mainly under air rich conditions. Furthermore, the experimental data are utilised to derive release functions for the relevant NOx precursors NO, NH3 and HCN. The release functions were implemented in an in-house empirical packed bed combustion model [15 and 16], which serves as a basis for the subsequent CFD gas phase simulation of N species conversion. Figure 10 shows the NO, NH3 and HCN profiles calculated with the hybrid and the hybrid-streak formation model. Generally, distinct areas can be observed, where the release of NO, HCN and NH3 takes place. NO is released in the air-rich zones at the beginning and the end of the fuel bed. NO is formed in regions of simultaneously high temperature and high concentrations of O and OH radicals [17 and 18]. The locations, where the NO has been released are in line with the high concentrations of O and OH radicals above the bed (see Figure 9). In contrast, NH3 and HCN are primarily released from the main in-bed devolatisation/gasification zone. These differences result from the local differences in the in-bed availability of oxidiser (see Figure 8), which in turn depends on the distribution of the primary air under the grate as well as on the in-bed thermal conversion processes. At the beginning and at the end of the fuel bed high in-bed availability of oxygen primarily leads to the release of the fuel-bound nitrogen in form of NO (see Figure 8), while NH3 and HCN are formed at low in-bed availability of oxygen in the main in-bed devolatisation/gasification zone. The distribution of the N-containing species in the gas phase results from the simultaneous formation and reduction processes, taking place in different regions of the combustion chamber and depending on many factors. Here, by taking into account the effect of the streak formation model, it can be seen that the spatial distribution of NO and NH3, specially, above the fuel bed are different (see Figure 10). These differences are mainly attributed to the different oxygen and radical (O and OH) concentrations that are influenced by the streak formation model (see Figure 8 and Figure 9). Figure 11 shows the NOx profiles predicted with the hybrid and the hybrid-streak model. Table 2 provides the NOx concentrations predicted with the hybrid and the hybrid-streak model in comparison with NOx emission measurements at boiler outlet. The results indicate that the prediction is improved with the hybrid-streak formation model. This can be argued with the more accurate prediction of the species mixing process above the fuel bed and, therefore, of the radicals, that are important for the NOx formation processes.

Figure 10: Iso-surfaces of HCN concentration [ppmv] (left), NH3 concentration [ppmv] (middle) and NO concentration [ppmv] (right) calculated with the hybrid model (top) and the hybrid-streak formation model (bottom)
Figure 11: Iso-surfaces of NO\textsubscript{x} concentration [mg/Nm\textsuperscript{3} d.b., 13 vol\% O\textsubscript{2}] calculated with the hybrid model (left) and the hybrid-streak formation model (right).

Table 2: Predicted NO\textsubscript{x} concentrations with the hybrid and the hybrid-streak formation model in comparison to measurements

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
<th>Deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment</td>
<td>[mg/Nm\textsuperscript{3} d.b., 13 vol% O\textsubscript{2}]</td>
<td>129</td>
<td>-</td>
</tr>
<tr>
<td>Hybrid</td>
<td>[mg/Nm\textsuperscript{3} d.b., 13 vol% O\textsubscript{2}]</td>
<td>141</td>
<td>9</td>
</tr>
<tr>
<td>Hybrid-streak</td>
<td>[mg/Nm\textsuperscript{3} d.b., 13 vol% O\textsubscript{2}]</td>
<td>125</td>
<td>3</td>
</tr>
</tbody>
</table>

4. Summary and conclusions

A streak formation model has been developed to account for the effects of gas streaks arising from the fuel bed on gas mixing and reactions. The streak formation model is based on a correlation between the local gas residence time and a mixing time in which the mixing time is the necessary time to reach the fully mixed condition above the packed bed. A mixing state definition was introduced in order to evaluate the degree of mixing and the fully mixed condition, respectively, above the packed bed. The gas residence time introduced in the streak formation model was obtained by solving a scalar transport equation. A series of packed bed CFD case study simulations has been carried out to derive the mixing time introduced in the streak formation model. The primary air velocity, volatile mass flow rate and number of particles (bed thickness) were identified as influencing parameters for the derivation of mixing time. The number of layers was considered as independent parameter since it had considerable influence on the mixing. Then, the effect of primary air velocity and volatile mass flow rate variations on the mixing were studied for a defined number of layers (5, 10 and 15 layers). The results showed a negligible effect of the volatile release rates on mixing. However, the primary air velocity and particle Reynolds number, respectively, had a significant effect on mixing. The particle Reynolds number definition was applied in terms of particle diameter and primary air velocity. This definition helped to reduce the number of independent parameters and to make the model applicable for any fuel particle size. The results of the CFD packed bed case study served as look-up table for the calculation of the mixing time in dependence of the different influencing parameters. The mixing time can be retrieved by a linear interpolation between the calculation points in dependence of the particle Reynolds number and the number of fuel layers. Furthermore, the application of the streak formation model has been verified for a pilot-scale grate furnace. Two simulations have been
performed, with and without the effect of the streak formation model. An in-house developed hybrid gas phase combustion model applicable for laminar to turbulent flow situations was used for both simulations (hybrid model). For the case that considers the effect of streaks on combustion, the particle Reynolds number and the number of layers (fuel bed thickness) have been calculated from the velocity profile specified by the empirical packed bed model as well as the assumed height of the fuel bed, respectively. The mixing time profile for the pilot-scale grate furnace was then evaluated by an interpolation through the values retrieved as a function of the particle Reynolds number and the bed height. Two scalar transport equations have been solved for gas residence time as well as mixing time to derive the local mixing function defined in the streak formation model. The effective reaction rate within the hybrid model was achieved by multiplying the mixing function, which considers macro-mixing, with the reaction rate predicted with the hybrid model. The results from the pilot-scale biomass grate furnace with and without the effect of streaks showed that in the present case, the streaks had no big influence on the combustion process including flue gas temperature and CO emissions. The low oxygen concentrations in the primary combustion zone and high flue gas residence time result in a full CO burnout at furnace exit as well as a full conversion of oxygen before the secondary combustion zone. However, the formation of reacting radicals (e.g. O and OH), especially, in the region above the bed are influenced by the streak formation model since the reaction progress is delayed caused by the incomplete mixing.

In the next step, NO\textsubscript{x} simulations have been performed in a post-processing approach based on the solution obtained from the combustion simulations. The NO\textsubscript{x} precursor species release profiles have been calculated with an empirical packed bed model. The distribution of the NH\textsubscript{3}, HCN and NO profiles showed that the streak formation model has a strong influence on the spatial distributions of the aforementioned species. This is mainly due to the slowdown of the reaction rate predictions caused by the streak formation model. Finally, the NO\textsubscript{x} emissions calculated with the streak formation model showed a better agreement with measured values due to the superiority of the model for the prediction of the reacting radicals above the packed bed. Concluding, the streak formation model in combination with the hybrid gas phase combustion model displayed a potential for an improved NO\textsubscript{x} prediction since it considers species mixing and reaction processes above the fuel bed with a higher accuracy. In the future, extensive validation simulations for real-scale plants are foreseen in order to validate and evaluate the model in more detail and for different framework conditions.

5. Literature

2. R. Scharler, E. Widmann, I. Obernberger CFD modeling of NO\textsubscript{x} formation in biomass grate furnaces with detailed chemistry A.V. Bridgewater, D.G.B. Boocock (Eds.), Science in thermal and chemical biomass conversion; Sept 2004, CPL Press, Victoria; Canada. UK (2006), pp. 284–300
5. Kilpinen P. pia.kilpinen@uku.fi or pia.kilpinen@abo.fi.


