CFD SIMULATIONS AS EFFICIENT TOOL FOR THE DEVELOPMENT AND OPTIMISATION OF SMALL-SCALE BIOMASS FURNACES AND STOVES

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The application of CFD simulations is gaining increasing importance for the development of furnaces and boilers. Despite the high complexity of the underlying processes, BIOS has developed a CFD model for biomass grate furnaces and successfully applied it for the development and optimisation of numerous plants of all scales. In this work, selected results from the simulation of continuously operated furnaces, wood log fired stoves and boilers, as well as results from CFD simulations of NOx and fine particle formation are shown in order to demonstrate the advantages and application possibilities of advanced CFD simulations for small-scale biomass combustion plants. The results show, that the CFD-aided technology development leads to reduced emissions, a better utilisation of the furnace volume, an increased fuel flexibility and an enhanced plant efficiency. Furthermore, CFD simulations result in reduced development times, test efforts and an increased security during plant development. Finally, a deepened understanding of the processes in biomass combustion plants is achieved. The applications of CFD models for small-scale plants show, that they are highly efficient tools for the development of new plant series.

Keywords: CFD, modelling, biomass, combustion, small-scale application

1 BACKGROUND AND CONTENT OF WORK

CFD simulations are applied for the 3D simulation and analysis of flow and heat transfer processes and, therefore, are applied for the development of furnaces and boilers. However, the simulation of biomass combustion plants is especially difficult due the highly complex and interacting processes of solid biomass combustion and turbulent reacting flow in the combustion chamber. Therefore, BIOS together with researchers of Graz University of Technology and BIOENERGY 2020+ has developed a CFD model for the development and optimisation of biomass grate furnaces (see [11] and [14]). The model consists of an in-house developed empirical fixed bed combustion model, which can also be applied for wood log combustion, as well as CFD models especially adapted and validated for turbulent reactive flows in biomass combustion plants. The applicability of the overall CFD model and the reliability of the simulation results were tested for a number of biomass combustion plants of all size-ranges (see [11], [17], [12], [14], [15], [19], [13] and [16]). Moreover, a new NOx formation model was developed [25] and a model for the formation of fine particles from ash forming elements is being developed [22] by BIOS in co-operation with Graz University of Technology and BIOENERGY 2020+

In the small size-range, BIOS has successfully applied CFD simulations for the support of the development of pellet boilers, wood chip boilers as well as new multi-fuel boilers for the combustion of agricultural residues. Furthermore, the in-house developed wood log combustion model enabled the successful development of new wood log fired boilers and stoves. In the present paper selected results from different case studies are shown in order to demonstrate the application possibilities and advantages of a CFD-aided development of small-scale boilers and stoves as well as the possibility to reduce NOx and PM1 emissions by primary measures by CFD simulations.

2 APPLICATION AND OBJECTIVES OF CFD SIMULATIONS

CFD simulations enable a 3D process analysis and hence an efficient technology and plant development and optimisation. The application of the simulation tool leads to reduced development times and costs and finally to an increased security during plant development. The objectives of a CFD-aided development and optimisation are:

- Emission reduction (CO, NOx, fine particles from incomplete combustion and from ash forming elements)
- Efficient air-staging ⇒ reduction of nitrogen oxides (NOx) via primary measures
- Good mixing of unburned flue gas with secondary air in the secondary combustion zone ⇒ low CO and fine particle emissions due to incomplete combustion
- Optimal exploitation of the furnace and boiler volume as a basis for a reduction of plant dimensions
- Reduction of excess air and increase of plant efficiency
- Reduction of local velocity and temperature peaks in order to reduce material erosion, ash deposit formation and fly ash emissions
- Evaluation of sensitivities (e.g. influence of load, water content, changes in air staging)

State-of-the-art CFD simulations open a broad range of application possibilities for continuously operated grate furnaces and wood log combustion plants in the small size-range in order to achieve these targets. CFD simulations of flue gas velocities and temperatures, material and surface temperatures of steel, refractory lining, insulation and glass panels, flue gas residence time distributions, pressure losses over different plant zones as well as CO and O2 concentrations are performed. Furthermore, fly ash particle trajectories are simulated as a basis for the calculation fly ash impaction rates on furnace walls and ash precipitation rates in different plant zones. NOx formation in the combustion chamber and NOx emissions can be calculated with an...
especially in-house developed NOx postprocessor model with detailed reaction kinetics. Simulations of fine particle formation and ash deposit formation are possible with a comprehensive model under development. The simulation results are then applied to support plant development and optimisation.

3 MODELS APPLIED

In the following, a brief overview about the models applied in the case studies is given.

3.1 Combustion of solid biomass on the grate

3.1.1 Basic empirical packed bed combustion model

An empirical model was developed for the description of solid biomass on the grate (see [11], [24] and [20]). This model describes the mass and energy fluxes as boundary conditions for the following CFD simulation of turbulent reactive flow in the combustion chamber. The empirical packed bed combustion model consists of 3 parts:

- 1D-profiles along the grate, which describe fuel drying and the thermal degradation of the fuel components C, H, O as well as profiles of primary air and re-circulated flue gas supplied below the grate are the basis of the model.
- By the definition of conversion parameters based on literature data and experiments, which describe the conversion of the fuel components C, H, and O to the flue gas components CH₄, CO, CO₂, H₂, H₂O and O₂ in dependence of the local fuel composition and the stoichiometric air ratio on the grate, the local composition of the flue gas released from the packed bed can be described.
- This enables the final calculation of the local mass and energy profiles and hence, the profiles of flue gas velocity, temperature and composition along the grate.

The results of the simulation applications (e.g. [11], [17], [12], [14], [15], [19], [13] and [16]), showed that the empirical packed bed combustion model is sufficiently accurate for the calculation of the boundary conditions for the CFD simulation of flow and gas phase combustion in the furnace. However, it is noted that the processes of solid biomass combustion on the grate can not be described by the empirical packed bed combustion model.

In order to overcome the shortcomings of this model, an advanced CFD model for packed bed combustion which enables the 3D simulation of solid biomass combustion on the grate in dependence of relevant influencing parameters like air staging, fuel water content and particle size is being developed in co-operation with BIOENERGY 2020+ [10]. The model consists of a layer model for thermally thick biomass particles with temperature gradients and a hybrid Euler/Lagrange multiphase approach for modelling of particle movement on the grate. Currently this model is being tested for different biomass grate furnaces.

3.1.2 Wood log combustion model

The empirical packed bed combustion model was modified especially for the combustion of wood logs in stoves and boilers, which are operated in a discontinuous batch mode [13]. Here, a time-dependent profile of wood log combustion is derived by the transformation of the release profile along the grate calculated by the basic packed bed combustion model. With the profiles as a function of time the composition of the evaporated water and the degraded fuel components C, H, and O can be calculated at any time. Furthermore, the mass and composition of the released flue gas can be calculated over the whole batch. Since an unsteady CFD simulation of the whole batch process is impossible so far, virtual steady-state operating conditions have to be defined. In order to reduce a possible falsification of the CFD simulations of the stove by the heat storage of the stove, an energy balance around the stove as a function of time has to be performed based on test run data. By this energy balance, two virtual steady-state operating cases with a heat storage of the stove, which is approximately zero, can be estimated.

In order to enable the simulation of the whole combustion batch and to reduce calculation uncertainties, the development of transient CFD simulations routines for batch combustion processes is planned as future application.

3.2 CFD simulation of gas phase combustion

For the simulation of the gas phase usually the Realizable k-ε Model for turbulence, the Discrete Ordinates Model for radiation, as well as the Eddy Dissipation Concept (EDC) ([4] and [8]), which is an extension of the Eddy Dissipation Concept (EDC) ([4] and [8]), which is an extension of the Eddy Dissipation Model (EDM) by Magnussen and Hjertager [9] in combination with a global Methane 3-step mechanism (CH₄, CO, H₂, CO₂, H₂O, O₂) [1] are applied. The sub-models as well as the gas phase models together with the empirical packed bed combustion model have been experimentally validated ([11] and [14]) and successfully applied for several plants. Additionally, residence time calculations of the flue gas in different zones of the plant as well as impaction rates of inertial particles on furnace and boiler walls and precipitation rates in different plant zones are calculated.

3.3 CFD simulation of NOₓ formation

In order to describe the release of the nitrogen components as boundary conditions for the simulation of NOₓ formation in the combustion chamber, the empirical packed bed combustion model was extended by the release of the most relevant NOₓ precursors HCN, NH₃ and NO, which depends on the local stoichiometry along the grate (see [24] and [23]). The release of these species is derived from lab-scale fixed bed batch reactor tests [23].

The EDM in combination with global reaction mechanisms is not able to describe complex interactions of turbulence and multi-step reaction kinetics as given in case of NOₓ formation in biomass combustion plants. Therefore, a NOₓ postprocessor model for biomass combustion plants was developed and validated (see [25]). The model consists of the Eddy Dissipation Concept (EDC) ([4] and [8]), which is an extension of the EDM and which allows for a consideration of the interactions of turbulence and complex reaction kinetics in combination with a detailed reaction mechanism (see [7] and [25]).
3.4 CFD simulation of fine particle and ash deposit formation

Ash related problems are of major relevance in biomass combustion plants. For small-scale plants fine particulate emissions and ash deposition are of special relevance. At BIOENERGY 2020+ in cooperation with Graz University of Technology and BIOS a flexible and comprehensive ash deposit formation model is currently being developed in order to allow for a prediction of ash deposit and fine particle formation in biomass boilers in dependence of fuel type and plant operation conditions ([22]).

At present, the model allows for the simulation of the time-dependent ash deposit formation and its influence on heat transfer in the boiler as well as the prediction of fine particle emissions. In order to describe the release of ash vapours and the entrainment of coarse fly ash particles from the packed bed as boundary conditions for the subsequent CFD simulation the empirical packed bed combustion model was extended (see [22] and [21]). The release rates of the ash forming elements are determined by ash mass balances over the plant investigated as well as by literature and lab-scale fixed bed batch reactor experiments. Additionally, the entrainment of the coarse fly ash particles is estimated by the ash mass balances. The model includes wall condensation of ash forming vapours using thermodynamic equilibrium calculations to determine the vapour pressures of the ash components. For the sulphur species, a kinetically limited reaction rate has been implemented. Furthermore, the model considers the deposit build-up by coarse fly ash particles. While the stickiness of salt-rich particles is determined by a melt approach, regarding silica-rich particles the viscosity of the particles is used. Brittle and ductile erosion models have been implemented in order to account the reduction of the layer thickness by the impaction of non-sticky particles.

Furthermore, the fine particle model includes sub-models for the formation (nucleation and condensation of ash vapours) and the deposition of the fine particles on the walls (thermophoresis and diffusion). Currently, the particles are described only by a single particle size class. An enhancement and further tests of the model are ongoing.

4 SELECTED CASE STUDIES

In the following, selected case studies concerning the CFD based design and optimisation of biomass combustion plants are shown. Case study No. 1 dealing with the optimisation of continuously operated boilers and case study No. 2 and 3 dealing with the optimisation of wood log fired boilers and stoves have the purpose to highlight the application possibilities and advantages of state-of-the-art CFD simulation techniques. Case study No. 4 with the CFD simulation of NOx formation and case study No. 5 with the simulation of fine particle formation are focussing on emission reduction and have the purpose to show new trends in CFD simulations and the potential and importance of CFD simulations for the support of the development of new highly efficient micro-scale, low-emission and multi-fuel furnace technologies.

4.1 Case Study No. 1: Design and optimisation of continuously operated boilers

The secondary air nozzles (and eventually the nozzles for tertiary air injection and the injection of re-circulated flue gas) are of special importance when designing and optimising the geometry of a furnace. The nozzles are a key factor in order to achieve good turbulent mixing and homogenisation of the flue gas, to reduce the furnace volume, to lower excess air (increased efficiency) and to provide an efficient air staging without backflow in the primary combustion zone (NOx reduction by primary measures). Furthermore, by an optimised secondary air injection, NOx can be reduced and flue gas velocity and temperature peaks can be lowered in order to minimise ash deposit formation and erosion.

As shown in Figure 1 for the basic variant, the flue gas velocity above the fuel bed is relatively high, which may lead to the dispersion of fuel and ash particles from the fuel bed. Furthermore, in the primary combustion zone (PCZ) no settling zone for the particles was detected. In the optimised variant the PCZ was enlarged (doubled cross-section above the grate). Even though the cross-section of the grate is the same as for the basic variant, the cross-section increases above the fuel bed surface. This leads to a reduction of the flow velocity through the fuel bed and should lead to a reduction of the entrainment of particles with the flue gas.

![Figure 1: Iso-surfaces of flue gas velocity (m/s) in a vertical cross-section trough the axis of the combustion chamber for the basic variant (left) and the optimised variant (right) of a 20 kW overfeed pellet boiler; nominal load](image-url)

**Figure 1:** Iso-surfaces of flue gas velocity [m/s] in a vertical cross-section through the axis of the combustion chamber for the basic variant (left) and the optimised variant (right) of a 20 kW overfeed pellet boiler; nominal load

**Modification:** larger cross-section of the PCZ and smaller cross-section of the secondary air nozzles

Furthermore, it is shown, that the entrance velocity of the secondary air jets is rather low in case of the basic variant. This leads to a poor mixing of the flue gas with air. In the optimised variant, the secondary air nozzle cross-section was reduced leading to a higher exit velocity of the jets and a higher penetration depth compared to the basic variant. Finally, by this measure an improved mixing with air and a break-up of streaks could be achieved, which in turn lead to an improved utilisation of the SCZ (average flue gas residence time t* in the SCZ is 0.14 s in case of the basic variant and 0.38 s in case of the optimised variant; see Figure 2).
As a consequence of the improved turbulent mixing and the utilisation of the SCZ the CO emissions predicted at the entrance to the fire tube boiler could be significantly lowered to 29 ppmv, wet flue gas, compared to 246 ppmv, wet flue gas, for the basic variant (Figure 3).

In Figure 4, a significant backflow of secondary air in the PCZ is shown for the basic variant of the depicted envelope of flue gas temperatures > 800 °C at the entrance to the fire tube boiler could be avoided by an increased nozzle diameter and a stronger radial direction of the nozzles. However, the exit momentum is high enough to mix the flue gas with air as a basis for a good flue gas burnout.

4.2 Case Study No. 2: Design and optimisation of wood log fired boilers

In the case of log wood boilers CFD simulations allow for an analysis of the penetration of the PCZ with primary air, the exploitation of the secondary combustion zone as well as the mixing of flue gas with secondary air and the CO burnout. Furthermore, it is possible to identify and reduce velocity and temperature peaks for a best possible avoidance of material erosion and ash deposition rate and, furthermore, to investigate the heat transfer in the boiler as a basis for an optimisation of the thermal efficiency. The pressure losses in different plant sections can be investigated as a basis for an optimised dimensioning of the fans.

In Figure 5 and Figure 6 exemplary results of the CFD simulation of a wood-log fired boiler are depicted. Figure 5 shows path-lines of the primary air, coloured by the gas temperature. By this simulation the quality of the penetration of the PCZ can be investigated and optimised, in order to achieve a good and even burnout of the wood logs and to avoid channelling and bridging. In Figure 6 the calculated CO concentrations in different cross-sections of the SCZ are illustrated. Obviously, via an optimised configuration of the secondary air nozzles (reduced nozzle number) and the secondary combustion zone (additional redirection of the flue gas) the turbulent mixing of flue gas with secondary air and the CO burnout are much better for the optimised geometry than for the basic geometry.
bypass flow and an insulation of the post combustion chamber. By these measures, the temperature in the post-combustion chamber was elevated and the CO burnout considerably improved. Moreover, the efficiency was improved by a considerably larger heating surface of the transition between the post-combustion chamber and the chimney.

A further improvement could be achieved by the optimised variant which was realised as testing plant. Here, additional tertiary air nozzles have been installed in the rear part of the combustion chamber, which lead to an improved flue gas burnout already in the combustion chamber. Moreover, the CO emissions are a leading parameter for the burnout quality of the flue gas and can be used as an important indicator concerning organic fine particle emissions from incomplete combustion. Besides the considerably reduced CO emissions also the organic fine particle emissions could be reduced (see [5] and [2]). Finally, the excess air could be reduced, leading to a higher plant efficiency.

### Table 1: Test run results in comparison with benchmark values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Test run</th>
<th>Benchmark value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO emissions</td>
<td>[mg/MJ]</td>
<td>429</td>
<td>750</td>
</tr>
<tr>
<td>OGC emissions</td>
<td>[mg/MJ]</td>
<td>15</td>
<td>50</td>
</tr>
<tr>
<td>Fine particle</td>
<td>[mg/MJ]</td>
<td>16</td>
<td>-</td>
</tr>
<tr>
<td>emissions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total dust</td>
<td>[mg/MJ]</td>
<td>18</td>
<td>20</td>
</tr>
</tbody>
</table>

In Table 1 results from comprehensive test runs with the optimised stove in comparison with benchmark values (values according to relevant emission limits) are shown. The measurements confirmed the predicted trends and showed that the emissions from incomplete combustion (CO, OGC) are considerably lower than the benchmark values defined. This shows that by means of the in-house developed wood log model CFD simulations can also be applied to efficiently support the optimisation of modern wood log stoves with increased efficiency and low CO and fine particle emissions.

### Figure 6: Iso-surfaces of CO concentrations [ppmv w.b.] in a horizontal cross-section (top) and the vertical symmetry plane (bottom) through the secondary combustion zone of a wood log furnace

**Modifications:** reduced number of secondary air nozzles; additional redirection in the SCZ; removed barrier at the entrance to the boiler

### Figure 7: Iso-surfaces of CO concentrations [ppmv w.b.] in the flue gas in the vertical symmetry plane of a stove

**Modifications:** closure of opening in the redirection baffle; additional tertiary air nozzles; larger transition to the chimney and insulation of the post-combustion chamber
4.4 Case Study No. 4: CFD simulation of NOx formation

The reduction of NOx emissions is of great relevance due to continuously stricter emission limits and due to the combustion of "new" agricultural fuels with enhanced nitrogen contents. To reduce NOx emissions effectively by primary measures it is important to operate at reducing conditions at sufficiently large flue gas residence times in the PCZ and gas temperatures of the bulk flow between 900 – 1100 °C. Therefore, false air and backflow of secondary air into the primary combustion zone (PCZ) have to be avoided. Additionally, it can be helpful to increase the size of the PCZ and the mixing of the flue gas in the PCZ, as well as to keep the flue gas temperatures at a moderate level (< 1500 °C) in order to avoid the formation of thermal NOx. A good mixing and temperature control can be achieved by flue gas recirculation besides cooled furnace walls. However, it has to be taken care that the temperature does not drop below 850 °C in order to allow for efficient NOx reduction. From Figure 8 it can be seen, that the formation and reduction of nitrogen oxides mainly takes place in the PCZ and in the region of the secondary air nozzles. Looking at the TFN/TFNin ratios it is possible to identify the regions of NOx reduction (the smaller the ratio, the more NOx precursors (HCN, NH3 and NOx) are reduced to N2). In the example shown below it can be seen, that NOx is mainly formed in the outer, oxygen-rich region of the PCZ and that it is reduced in the inner, oxygen-lean region of the PCZ.

Figure 8: Iso-surfaces of NOx concentrations [ppmv w.b.] (left) and of the local TFN/TFNin ratio [-] (right) in a vertical cross-section through the axis of a 20 kW underfeed multi-fuel boiler at nominal load
Explanations: fuel: straw; fuel-N = 0.54 wt.% d.b.; \( \lambda_{\text{air}} = 1.71; \) \( \lambda_{\text{fuel}} = 0.69; \) TFN (total fixed nitrogen): sum of all moles of nitrogen contained in NO, NH\(_3\), NO\(_2\), HCN and N\(_2\)O; TFN/TFNin: TFN in the flue gas related to TFN released in the fuel bed and introduced via the recycled flue gas (TFNin).

4.5 Case Study No. 5: CFD simulation of fine particulate formation

The reduction of fine particle emissions is presently one of the key issues in the development of new small-scale plants. Thus, BIOENERGY 2020+ in co-operation with BIOS is developing a comprehensive CFD model for the simulation of ash deposit and fine particle formation, which can already at the present state of development serve to investigate the local formation of fine particles in the boiler in dependence of relevant influencing parameters and thus can be applied as process optimisation tool (for the design of low-dust combustion technologies).

During the combustion of biomass on the grate, ash forming vapours are released. Due to the cooling of the flue gas in the boiler, fine particles are formed by nucleation and, furthermore, ash vapours condense on the particles formed. In parallel to fine particle formation, the vapours condensate on the cooled boiler walls when the vapour pressure at the wall is lower than in the flue gas boundary layer. To describe the fine particle formation, all the processes involved (chemical reactions including sulphur kinetics, direct wall condensation, as well as fine particle formation and deposition) are considered by the in-house model under development.

In Figure 9 and Figure 10 the simulation results for a 70 kW pellet boiler are shown. In the PCZ, the flue gas temperature and the wall temperatures are too high for a direct wall condensation or fine particle formation. The first formation was predicted at the exit of the PCZ.

Figure 9: Total fine particle concentrations [mg/Nm³ dry flue gas, 13% O2]; (left) and chemical composition of the fine particles (right)
Explanations: 70 kW pellet boiler; 1…first particle formation; 2…particle formation starts to dominate at the entrance into the heat exchanger

Simultaneously to the fine particle formation, condensation occurs at the cooled walls. The highest deposition mass fluxes have been calculated on the opposite side of the SCZ. In this region, mass transfer coefficients as well as concentration gradients at the wall are high in comparison to the other regions. In the heat exchanger, the condensation flux strongly decreases and the formation of fine particles dominates. For the purpose of model check, the simulation results have been compared with measurements during test runs. The predicted fine particle emissions are in good agreement with the measurement values (simulated: 9.92 mg/Nm³; measured: 7.65 mg/Nm³).
Moreover, as shown in Figure 9, the predicted chemical composition of the fine particulate emissions is in good agreement with results from chemical analyses. Concluding, the selected results of a number of validation simulations showed that already at the present state of development the model is able to predict fine particulate formation and emissions even at a quantitatively acceptable level. Hence, the model under development can be already applied as efficient tool for the development of new low-dust combustion technologies since it predicts local fine particle formation in dependence of relevant influencing parameters and thus leads to a better and deepened understanding of the underlying processes.

5 SUMMARY AND OUTLOOK

In this paper an overview about the far reaching possibilities of CFD simulations for small-scale biomass combustion plants is given in a number of case studies. Selected results for automatically operated plants and wood log fired boilers and stoves are presented. Furthermore, results from in-house developed and highly innovative CFD models for NOx formation and the formation of fine particulates are presented. Concluding, it is stated that the CFD simulations are an efficient tool to develop new plants with reduced emissions (CO, NOx, and particles) and increased plant efficiencies as well as new multi-fuel plants for the combustion of agricultural fuels. Finally, the simulations lead to reduced plant development cycles and testing efforts and, furthermore, to a higher safety during the plant development due to a better and deepened understanding of the fundamental processes in the plant.

Furthermore, these new and innovative CFD models are being developed in order to enhance the capabilities of the simulation routines and to link the models with the final aim to develop a comprehensive model, describing all relevant processes in biomass combustion plants ("the virtual biomass combustion plant") to supply a powerful tool for the development of new technologies.

One interesting development is the speed-up of the time-consuming NOx simulations by the application of the chemical cell agglomeration algorithm [3]. In the field of ash deposit and fine particulate formation modeling [22], further research work is ongoing concerning the validation of the models with experimental results as well as the further development of the stickiness models for coarse fly ash particles based on drop tube experiments and the fine particle model with the consideration of a particle size class instead of an average particle size. A highly innovative development is a CFD model for the 3D simulation of the combustion of the solid fuel on the grate in dependence of relevant influencing parameters [10]. Currently this model is being linked with a layer model for thermally thick biomass particles with temperature gradients inside the particle allowing parallel progress of the sub-processes drying, devolatilisation and char burnout and tested for real-scale applications.

6 REFERENCES

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