MODERN SIMULATION TOOLS AS A SUPPORT FOR THE DEVELOPMENT AND OPTIMISATION OF AN INNOVATIVE BALED BIOMASS-FIRED COMBUSTION CHAMBER

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ABSTRACT: The present work shows that the joint application of modern simulation methods like process simulation and computational fluid dynamics (CFD) is a powerful tool for the design and optimisation of complex and innovative concepts in the chemical engineering practise. The application of these tools to the presented concept of a baled biomass-fired combustion chamber allows for the optimisation of operation parameters and detailed engineering of the combustion apparatus. The major goals are the maximisation of the thermal efficiency and the reduction of gaseous and particulate matter emissions. To meet these goals it is very important to have precise mathematical models with sharpened model parameters available. Therefore the model approaches have been validated and refined using results from extensive combustion experiments conducted at an existing 2MW pilot plant. Several modelling approaches are presented especially focussing on the treatment of heterogeneous combustion and the prediction of gaseous emissions such as nitrogen oxide. With validated models on a sound physical basis both process simulation and computational fluid dynamics allow for a significant reduction of the development costs and the time-to-market of innovative chemical engineering concepts.
Keywords: solid biofuels, combustion, emission reduction

1 INTRODUCTION

The use of biomass in combustion processes for the production of heat and power is of increasing interest because of its CO2-neutrality. The development of appropriate designs of combustion systems for these fuels is rather challenging, often time-consuming and cost-intensive due to the heterogeneous composition and disadvantageous ash melting behaviour of biomass. The application of modern simulation tools like process simulation or computational fluid dynamics (CFD) offers the possibility to reduce development costs and the time-to-market of the mentioned combustion concept and the enclosed devices.

Within the present work these simulation tools were applied during the development of an innovative combustion system for the generation of heat and electrical power by combusting baled biomass. For the achievement of reliable results several modelling approaches (e.g. for the time-dependent turbulence effects, the radiative heat transfer, homogeneous gas reactions and the turbulence-chemistry coupling, the heterogeneous biofuel, the solid fuel combustion and for the formation of NO_x-emissions) had to be combined. In addition to the simulations extensive combustion experiments were carried out at an existing medium scale pilot plant of 2MW thermal power.

The collected experimental data were compared with the simulation results and were used for adjusting the simulation models and parameters. With this validated modelling approach the optimisation of combustion parameters as well as the design of the combustion chamber could be done. The major goals are the maximisation of the thermal efficiency of the combustor and the minimisation of carbon monoxide, nitrogen oxide and particulate matter emissions. The optimisation of residence time distributions, the mixing behaviour of the hot reaction gas with secondary air and the investigation of the temperature distribution inside the analysed device using computational fluid dynamics have proven to be valid measures for emission reduction.

2 MODEL IMPLEMENTATION

2.1 Process simulation

A flowsheet of the combustion pilot plant as it was modelled in the process simulation is shown in Figure1. The outer shell of the combustor was modelled as an adiabatic wall and the combustion was assumed to be complete.

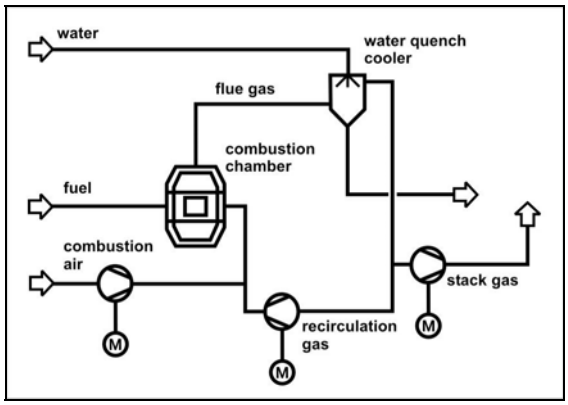

Figure 1: Simplified flowsheet of the 2MW pilot plant

Since no carbon monoxide emissions can be calculated in the used process simulation model, this has to be done by using the real flow behaviour of the reaction chamber calculated with CFD. Contrary to that a simplified model for the prediction of nitrogen oxide emissions has been developed. A detailed description of this model is given in [1] and [2]. This model uses the overall stoichiometric ratio for the calculation of the nitrogen oxide emissions. This parameter is rather easily accessible through measurements of the flue gas oxygen content and fuel mass flow. Although the current combustion concept takes advantage of the principle of air staging it is not necessary to use the stoichiometric ratio of the primary combustion zone if optimal air staging conditions can be assumed. Due to the low combustion temperatures, which are caused by intensive

flue gas recirculation, the generation of thermal nitrogen oxide is negligible. According to [3] also the generation of Prompt NO_x can be neglected. Thus Fuel-NO_x is the only relevant formation mechanism for the current application.

2.2 Computational fluid dynamics (CFD)

A short introduction to the applied models is given here; a more detailed description of the models, their development routines and their parameter optimisation has recently been published ([2] and [4]).

In a first step the given combustion chamber geometry (as it can be seen in Figure 2) has been discretised into approximately 1.500.000 finite volume cells. For this task the geometrical pre-processor GAMBIT™ V2.1 has been used. The computational mesh has been imported into the commercial CFD-solver FLUENT™ V6.1 (see [5] for details), where the stationary calculations have been accomplished. This solver is based on Reynolds-averaged Navier-Stokes equations (RANS) that are solved in an iterative process.

The boundary conditions of mass flows, temperatures and gas compositions for the different inlet zones of the CFD-model have been taken from process simulation results that balanced the data gained from the combustion experiments.

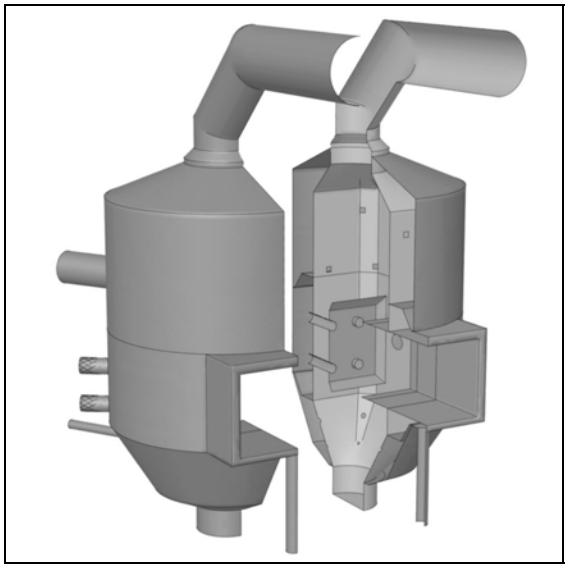

Figure 2: Geometry of the pilot plant combustor

For the modelling of the unsteady turbulent effects the so called SST-k-ω formulation (published by Menter [6]) has been used which has proved its applicability in several preliminary works (see [7] and [8]). The DTRM radiation model was used to simulate the heat transfer due to radiation because of its ability to handle optically thick media.

Concerning the description of homogeneous gas reactions two separate mechanisms have to be considered. The chemical reaction rate is modelled using a power law in terms of reactant concentrations and an Arrhenius approach in terms of temperature. This is a widely accepted proceeding in chemical reaction engineering. The transport of reactants to the site of reaction results from mass convection and diffusion. The convective part is solved together with the solution of the flow field. The diffusive mass transfer contains laminar diffusion (using Diffusion coefficients and Fick´s laws) and turbulent diffusion that is calculated using turbulence parameters generated by turbulence modelling. In turbulent flows (like in the current application) the turbulent diffusion is several magnitudes faster than laminar diffusion. For a correct description of the chemical conversion both reaction rate and reactant transport have to be combined. In the current work the so called eddy dissipation/finite rate approach has been applied. The speed of both mechanisms is calculated here but only the slower one is included in the chemical conversion whereas the faster one is assumed to be infinitely fast. This approach decouples the stiff differential equations resulting in lower computational effort and higher numerical stability. A full coupling of both mechanisms (chemical reaction and mixing rate) is also possible in FLUENT using the Eddy Dissipation Concept (EDC). This model is based on the assumption that the reaction time scales can be related to the dissipation of turbulent eddies which contains the reactants and products. A detailed description of this modelling approach is given in [9].

The solid biomass bale was modelled as a porous medium with homogeneous volume sources of various gaseous species as well as volumetric heat sinks (evaporation of humidity) and heat sources (char burnout). The evaporating gaseous species are: H_2O (bale humidity), CO and CO_2 from the char burnout, a pseudospecies called volatiles representing the volatile components of the solid biomass and finally several N-species as NO_x-precursors.

To simulate the NO_x-chemistry during combustion a formulation was applied for the conversion of fuel-N to nitrogen oxide. Because of the low occurring combustion temperatures (lower than 1200°C) the thermal NO_x formation is assumed to be negligible (see [3]). During the heterogeneous combustion steps (devolatilisation and char burnout) the fuel-bound N is converted to a mixture of the gaseous species NH_3, HCN, NO and N_2. The composition of this mixture has been studied recently (see [10]) for several solid biofuels. These gaseous species are in a first step assumed to evolve homogeneously over the bale volume. The NO_x-precursor species NH_3 and HCN are further exposed to homogeneous gas reactions with oxygen and nitrogen oxide. The kinetics of these reactions has been modelled using a global Arrhenius approach; the parameters were taken from literature (for NH_3 from [11] and for HCN from [3]). A schematic depiction of this NO_x-model is given in Figure 3.

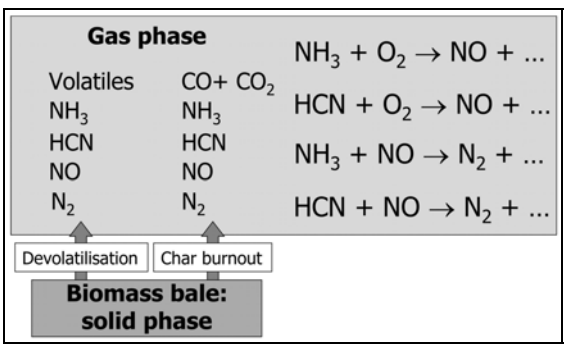

Figure 3: Illustration of the simulation model of the conversion of fuel-N to nitrogen oxide

3 RESULTS AND DISCUSSION

The first fundamental result of the CFD calculation is the flow pattern inside the computational domain. To give a short overview of this flow field contour plots of the gas velocity on several horizontal cross-sections of the combustion chamber are given in Figure 4.

The high gas velocities and the high degree of turbulence in the primary combustion zone induced by the primary air nozzles are clearly distinguishable. The addition of secondary air in the upper post-combustion zone and in the lower afterburning grate can also be seen. Based on this flow field an analysis of the residence time spectra can be done. In combination with the temperature field and the mixing behaviour this analysis allows for the quantification of the carbon monoxide and fly ash burnout. Additionally an attentive analysis of the flow field helps to locate flow dead zones and large scale vortices that result in unwanted back mixing. Thus the combustion chamber can be tailored to the essential dimensions without expensive experimental evaluation.

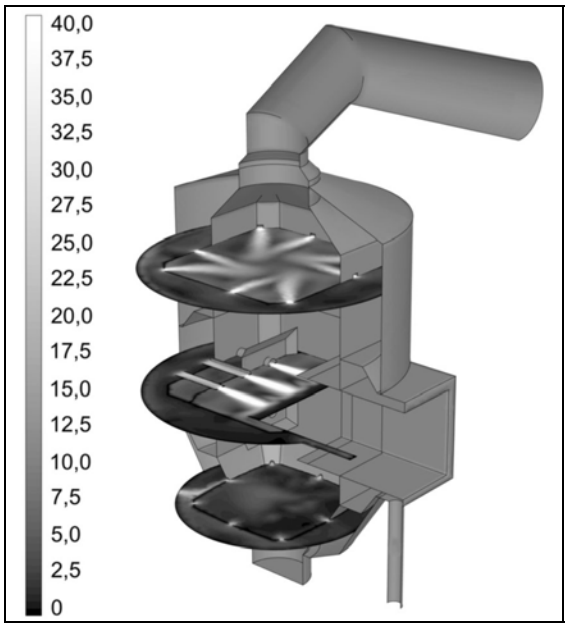

Figure 4: Contours of gas velocity magnitude on several horizontal cross-sections of the combustor (0 to 40 m/s)

Besides of the optimisation of the constructive details of the combustion chamber the choice of the proper steel grade for each part is of vital importance. A helpful tool for this task is the careful analysis of the temperature field inside of the combustor and especially the wall temperature distribution. In Figure 5 a depiction of the calculated wall temperatures of the combustion core is given. This picture also allows for the identification of "hot spots" in the combustion chamber where danger of slagging and high temperature corrosion can be expected. A variation of constructive details can easily be done.

For the evaluation of the quality of the NO_x-models applied in process simulation and CFD several variation calculations have been accomplished. The simplified NO_x-model has been used together with process simulation to predict the nitrogen oxide emissions over a wide range of the overall stoichiometric ratio. The results of these calculations can be seen as a continuous line in Figure 6.

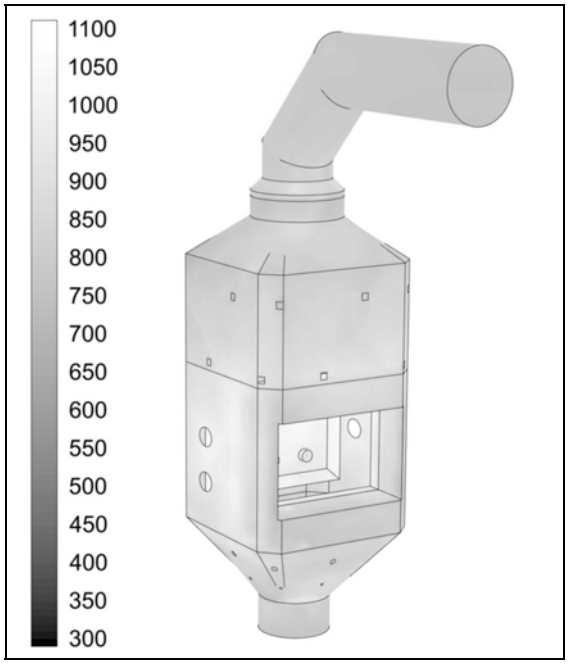

Figure 5: Wall temperature of the combustion core (300 to 1100 K)

At a constant stoichiometric ratio of 1,743 which represents approximately the basic combustor layout a set of CFD calculations have been accomplished. In these CFD cases the intensity of air staging has been varied. This was done by a shift of combustion air from the primary zone to the upper combustion zone. The results of these calculations can be seen as black triangles in Figure 6. The calculation results are accompanied by experimental data over the whole range of the stoichiometric ratio which are displayed as black dots in this diagram. The agreement of the predicted and the measured values is remarkable for both the process simulation results and the CFD results.

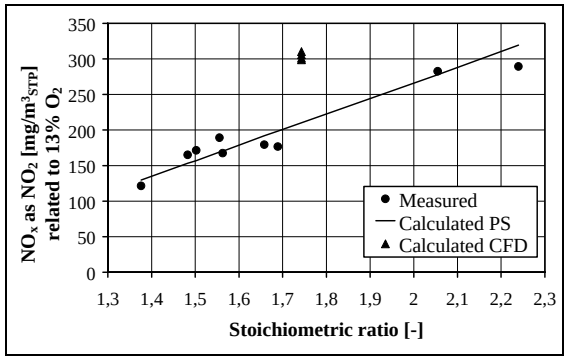

Figure 6: Measured and calculated nitrogen oxide emissions as a function of the overall stoichiometric ratio

A detailed analysis of the nitrogen oxide emissions calculated with the CFD-model showed only a very weak correlation between the intensity of air staging and the NO_x emissions. This fact can easily be seen in Figure 6 where the results of the four calculated operation conditions are situated in immediate vicinity. The operation conditions that have been studied are located in a range of 1:1,5 to 1:2,125 of the combustion air/recirculation gas ratio of the primary combustion zone. Typical experimental values are within this range

and the experimental results showed rather strong correlation of air staging intensity and NO_x emissions. It can be assumed that the deviation of the CFD results from this behaviour is caused by the applied simplification in the modelling approach for the turbulence-chemistry interaction. With the application of the EDC-model an enhancement of these results can be expected. Nevertheless the agreement of the absolute value of nitrogen oxide emissions is remarkable especially when the simplicity of the applied model is taken into account.

4 OUTLOOK

To improve the accuracy of the simulation results the model parameters need to be sharpened using more experimental values with higher precision. Therefore several modifications in the measurement system have been recommended and are currently in the state of implementation.

Furthermore the combustion apparatus will be implemented into a combined heat and power plant that produces steam for the generation of electricity and district heat. The process simulation of this complete cycle will be one of the next ambitious steps. With the generation of new flow boundary conditions the CFD calculations for this complex plant will also be possible.

For an improved significance of the CFD results several models will be refined. The most important revision will concern the characterisation of the solid biomass bale. The impressing of devolatilisation- and evaporation-profiles will be done by using user-defined functions. The modelling approach for the flow resistance and the thermal behaviour of the porous biomass bale will be improved based on experimental results and analytical considerations. The calculation of the gaseous emissions will be refined using the EDC formulation for the turbulence-chemistry interaction. The burnout and emission of fly ash particles will be treated using an Euler-Lagrange approach with defined drag and combustion characteristics.

With these improved models on a sound physical basis the future simulation works will especially focus on the prediction and reduction of gaseous and particulate matter emissions. Furthermore the burnout on the bale surface will be studied and constructive and operational innovations shall be developed to increase the burnout quality and the thermal output of the combustion unit.

5 CONCLUSIONS

The results of the present work show that the joint application of modern simulation methods like process simulation and computational fluid dynamics is a powerful tool for the design and optimisation of complex and innovative concepts in the chemical engineering practise. The application of these tools to the presented novel concept for the combustion of baled biomass allows for the optimisation of design parameters of the combustion chamber as well as the optimisation of various operation parameters. The major goals are the maximisation of the thermal efficiency and the minimisation of carbon monoxide, nitrogen oxide and particulate matter emissions of the combustion pilot plant.

It is very important to have precise mathematical models with experimentally validated and sharpened model parameters at hand to meet these above mentioned goals. Because of some simplifications in the modelling approaches that are necessary due to computational limitations all models show a limited range of applicability. The simulation engineer is requested to check for the applicability of a distinct model and should always challenge the significance of the gained results.

6 REFERENCES

[1] Kerschbaum A., Friedl A., Pfeffer M., Beckmann G.; Proceedings of the 2nd World Biomass Conference – Biomass for Energy, Industry and Climate Protection, Vol 2 (2004) 1397.

[2] Miltner M., Kerschbaum A., Jordan C., Harasek M., Friedl A.; Chemical Engineering Transactions, Vol 7 (2005) 345.

[3] Hill S.C., Smoot L.D.; Progress in Energy and Combustion Science 26 (2000) 417.

[4] Harasek M., Miltner M., Jordan C., Friedl A.; Proceedings of the 2nd World Biomass Conference – Biomass for Energy, Industry and Climate Protection, Vol 2 (2004) 1391.

[5] FLUENT 6 User's Guide, FLUENT Inc., 2001

[6] Menter F.R.; AIAA Journal, 32 (1994) 1598.

[7] Jordan C., Miltner M., Potetz A., Harasek M.; Chemie Ingenieur Technik 77 (8) (2005) 1061-1062 (in German).

[8] Miltner M., Jordan C., Potetz A., Harasek M.; Chemie Ingenieur Technik 77 (8) (2005) 1062-1063 (in German).

[9] Magnussen B.F., Hjertager B.H.; 16th International Symposium on Combustion, The Combustion Institute (1976).

[10] Winter F., Wartha C., Hofbauer H.; Bioresource Technology 70 (1999) 39.

[11] Brink A., Kilpinen P., Hupa M.; Energy & Fuels 15 (2001) 1094.

7 ACKNOWLEDGEMENT

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