Final report: Improved Bio-CFD Simulations

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Final report: Improved Bio-CFD Simulations

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Abstract
This report shortly describes the performed studies and the results of the project ‘Improved bio-CFD simulations’. The project objectives were to improve biomass particle conversion models such that they can be used in CFD calculations of biomass flames, and to provide better predictions of biomass particle conversion in PF boilers. Project activities have included development of biomass particle devolatilisation models, performing drop tube devolatilisation experiments with particles from 0.6 to 1.5 mm, performing a comparison of in-flame measurements and CFD modelling of a 30 MWth wood bio-dust flame and conducting a short review of the industrial implications of the conducted wood particle conversion studies.

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1.0 Introduction

The use of biomass on Danish PF (Pulverized Fuel) power plants have in recent years been done to reduce the use of coal, and thereby reduce net greenhouse gas emissions. Several collaboration projects dealing with PF firing of biomass with participation from Ørsted Bioenergy & Thermal power and the CHEC research group at Department of Chemical Engineering have previously been conducted [1,2]. This project is a continuation of those projects and was conducted in the period 2016 to 2019.

The project was a collaboration project with participation of Ørsted Bioenergy & Thermal power, BWSC, Rambøll, and DTU. The DTU activities of the project was funded by Nordic Five Tech (N5T) PhD grant, Ørsted Bioenergy & Thermal power and DTU. Regular project meetings with participation of all project partners were conducted in the project period.

Many biomass studies have dealt with combustion resembling the conditions in wood stoves, grate or fluid bed boilers. However, the conditions in PF boilers are somewhat different with local temperatures up to 1600°C, maximum residence times of less than 5 seconds and the use of wood particles with a maximum size of 3 mm. In this project the main activities have been directed towards obtaining an improved understanding of wood particle combustion at PF boiler combustion chamber conditions.

The project objectives were to improve biomass particle conversion models such that they can be used in CFD calculations of biomass flames, and to provide better predictions of biomass particle conversion in PF boilers.

The following project activities were conducted

A. Different biomass particle conversion models were developed. This included an empirical model for determining char yield, a 1D model for determining devolatilisation of non-spherical particles at high temperatures and a simplified 0D devolatilisation model that is well suited for implementation into CFD models. This work was conducted as a PhD project (Chapter 2).

B. A drop tube reactor was modified to study the devolatilisation of biomass particles in the size range of 250 µm to 2 mm. An experimental procedure was developed and the obtained experimental devolatilisation data was compared with the developed 0D devolatilisation model. The activity was partly conducted by two Master student projects (Chapter 3).

C. A CFD modeling of a 30 MW flame on a biomass fired boiler was performed and the results compared with in flame measurements made in previous study [3], (Chapter 4).

D. A short review on the status regarding our understanding of biomass particle conversion with respect to burn out in biomass PF boilers was conducted (Chapter 5). In this chapter is also included a short resume of two papers [Enclosure 3, 4] that was not made in this project but covers important aspects with respect to biomass particle combustion modelling.

As part of the project educational activities one PhD and two Master projects were conducted.
2.0 PhD study on modelling bio-dust combustion in suspension fired boilers

A PhD project dealing with development of models of particle devolatilisation at PF conditions was conducted. The project have provided verified models that can be applied to describe devolatilisation of biomass particles in biomass PF boilers, and two journal papers have been published and one is submitted [Appendix A 1-3].

The char yield from biomass determined from standard proximate analysis is typically in the range of 16 to 20 wt% db. However, at high heating rate particle conditions, such as they appear in PF boiler chambers the obtained char yields are much smaller, and can be down to 2 wt% daf. This can have a large influence on the combustion conditions in biomass PF boilers, since this will lead to a very high fraction of the combustion and heat release happens in gas phase, while only a small fraction of the energy is released by char combustion.

An equation for biomass char yield at PF conditions was determined by using least square fitting, and it is thereby possible to predict the char yield for wood and herbaceous biomass [Paper in appendix A1]. The model input parameters are heating rate, mean particle size, maximum local temperature and biomass potassium content. The model is validated against experimental data from the literature. An example of predicted and measured char yields are shown in figure 1. Independent data sets of wood and straw are predicted with an average error (RMSEP) of 0.9 wt% point daf.

Figure 1. Measured char yield versus modelled char yields for two wood species. [From Appendix A1]

To include herbaceous biomass, the model introduces a potassium cut of level at 0.53 wt % db, because the catalytic effect of potassium on the devolatilisation process levels off above this concentration. The equation with the determined parameters is shown in equation 1.

\[
CY_{\text{biomass}} = 10^{(3.437 + 0.685 \times KC - 0.6598 \times \log(FT) - 0.2130 \times \log(HR))} \quad \text{Eq1.}
\]

CY is the char yield in wt %daf, FT is the final temperature in K, HR is the heating rate in K/s, and KC is the potassium content wt %db; if KC > 0.53 wt %db, then KC = 0.53 in equation 1 is used. The work shows that increased potassium concentration increases char yield while increased heating rate and increased maximum temperature decrease the char yield. High heating rate and high final temperature leads to a faster release of
the volatiles and thereby probably minimize the formation of secondary char. Potassium catalyze the formation of char and thereby leads to higher char yields.

Models of coal devolatilisation at PF boiler conditions have been available for many years; however, models that can predict biomass particle devolatilisation at PF conditions are still scarce. Biomass particles differs from coal particles used in PF boilers by typically being much larger (0.05 – 3 mm) and in the case of wood particles having a typical aspect ratio of (AR = L/dp) of 2 to 3. Model for coal particles have often assumed an isothermal zero dimensional (0D) spherical particle. A 1D model including the effects of heat transfer and kinetics that can account for the influence of size and morphology on devolatilisation of biomass particles was developed [Appendix A2]. The model predictions was tested with experimental data from three published experimental studies. A flow reactor test using 79 µm particles [4], a single particle reactor study using 3 mm spherical particles [4] and a single particle reactor study using 9.5 mm spherical and cylindrical particles [5]. In Figure 2 is shown an example of a comparison of 3 mm spherical particles measured and modelled devolatilisation times. Generally was observed a reasonable prediction capability of the model for the for particles sizes (dp = 79 µm up to 9.5 mm), temperatures from 1276 to 1667 K and changes in particle aspect ratio.

Figure 2. Comparison of modeled devolatilisation time and measurements of 3 mm spherical particles of different density [From Appendix A2]. Experiments was performed on a single particles reactor with a gas temperature 1487 K and a wall temperature of 1187 K.

A parameter test was performed with the model to investigate the influence of aspect ratio, size, gas temperature, particle density and biomass moisture content on devolatilisation time. An example, the influence of changes in moisture content can be seen in Figure 3. It is seen that the onset of volatile release is delayed for particles containing higher moisture content. The model results show that the time for full devolatilisation varies more than two orders of magnitude in the relevant particle size range (dp = 0.08 – 3 mm). For the relevant gas temperature (Tg = 1300 – 1900 K) and density variations (ρ = 400-1000 kg/m³) devolatilisation time changes of a maximum factor of 2 is observed. Variations in moisture content primary influence the time for onset of devolatilisation, which may affect ignition and flame stability in suspension fired boilers. Changing
the aspect ratio from a sphere up to a cylinder with AR = 8 at constant radius only led to an increase in devolatilisation time of approximately 30%. A sensitivity analysis of the influences in changes of the model input parameters showed that changes in devolatilisation kinetics resulted in a larger relative change in devolatilisation time for the smallest particles, while changes in biomass thermal conductivity lead to a large influence on devolatilisation time for the larger particles. Further more one set of devolatilisation kinetics and heat transfer material properties could be used to simulate all the investigated cases; indicating that as long as size, form and density is correctly specified different wood types devolatilisation conversion can be correctly predicted with no change of other model input parameters.

Figure 3. Example of results from a parameter study with the devolatilisation model [From Appendix A2]. Influence of changes of biomass particle moisture content on devolatilisation conversion as a function of time for a particle with a diameter of 1.5 mm, an aspect ratio of 5 and exposed to an environment with a temperature of 1600K.

The developed 1D model of the biomass particle devolatilisation do use significant computer resources to calculate the conversion as a function of time. When being used in CFD calculations where repeated calculations of many particles is needed this is detrimental. A simpler 0D model was therefore developed [Appendix A3]. The 0D model employs Arrhenius parameters in a single first order devolatilisation reaction where the effects of kinetics and heat transfer limitations are lumped together. In this way, a biomass particle devolatilisation can be modelled as a zero dimensional isothermal particle facilitating the use for CFD modelling. The model was developed by calculating the devolatilisation conversion times using the 1D model for a range of conditions relevant for PF firing. The best fit for the 0D model with respect to changes in activation energy and pre-exponential factor was the found for the single cases. Then by statistical analysis equations that determine activation energy (E) and pre-exponential factor (A) as a function of aspect ratio, particle density, maximum gas temperature and particle radius was provided. The equations then determines the value of E and A that shall be used in the 0D model at the prevailing conditions. The 0D model can predict devolatilisation times for conditions in the parameter ranges; radius (40 – 1600µm), density (700 – 1300 kg/m³), gas temperature (1300 – 1900 K) and aspect ratio (1 – 8). The developed 0D model is well suited for use in CFD modelling.
3.0 Experimental study on devolatilisation on a drop tube reactor

Experimental data on wood devolatilisation are mainly available from entrained flow reactor tests with particles below 0.25 mm, or from single particle reactors using particles of 3 mm or larger. However, the wood particle input to biomass PF power plant burners are typically dominated by particles in the size range from 0.1 to 2 mm. It was therefore desirable to generate some experimental conversion data for biomass particles in the size range of 0.25 to 2 mm. Therefore, a new measuring procedure was developed, and devolatilisation measurements were conducted using a drop tube reactor [For details see enclosure 2]. Furthermore, a comparison of the developed 0D model with measuring data was performed.

When the project was started, a new drop tube reactor was available. However, the necessary equipment for performing devolatilisation experiments and a procedure for conducting such experiments was not developed. An overview of the drop tube reactor system after modifications are shown in Figure 4 and 5. On top of the reactor, a small injection system is mounted, whereby a small amount of biomass particles (from 1 g to 10 g) can be injected into the reactor through a ceramic pipe (diameter 10 mm) into the flow reactor. Below the reactor, a cooled collection system containing a collection chamber, a cyclone and a filter is located. The reactor is made of two ceramic tubes forming an outer annulus that is used for preheating the inlet gas, and a central pipe acting as pyrolysis reactor. The heated zone, where pyrolysis takes place, is 700 mm long and can be heated to a maximum temperature of 1400 °C. The conducted reactor modifications included construction and mounting of the particle feeding system and mounting of the double ceramic tube system that ensure a uniform temperature in the reactor.

Figure 4. Process and Instrumentation diagram for the Drop tube reactor [from enclosure 2].
Figure 5. Drawing of the top part of the drop tube reactor with the cooled top flange and the inner ceramic tube used for particle injection [from enclosure 2].

Figure 6. Comparison of volatile release with the 0D model and experimental results from drop tube devolatilisation experiments (0D model from appendix 3). Residence times was calculated by CFD to be from 0.6 – 1.1 s. Devolatilisation experiments was conducted at temperatures from 1000 to 1300 °C and particle sizes from 0.6 to 1.7 mm (determined by sieving). [from enclosure 2].

Some effort was directed to develop an experimental procedure for conducting the experiments, where particle pyrolysis conversion level could be determined as a function of temperature and particle size. Because of the low ash content of wood and the often unknown ash volatilization degree using of the ash as a tracer for determining devolatilisation degree was renounced. It was therefore decided to try to make a direct
determination of the degree of pyrolysis based on the number of collected particles and their weight. It was realized that it was impossible on the set up to collect very small particles in this manner so the methodology was tested with pine particles between 0.6 to 2 mm. For the smaller particles (below 1 mm), a lower collection efficiency and some fragmentation of particles was observed. The fragmentation can probably be attributed to the fast release of volatiles for the particles that experience a high heating rate, and thereby, the volatiles may induce a high internal pressure that leads to fragmentation. An improved particle collection method may improve the quality of the experimental data. In order to improve the understanding of the particle behavior in the reactor and determine particle residence times, 2D CFD simulations of the drop tube reactor were performed. An increased average residence time from 0.6 to 1.1 seconds was observed as particle size decreased. Experiments were performed by injecting 50 particles (of similar size), five injected at once, and then the solid yield was determined by direct weight measurement and taking the number of collected particles into account.

Devolatilisation experiments were conducted at temperatures from 1000 to 1300°C and compared with a simulation using the 0D model, as shown on Figure 6. It is seen that there is reasonable agreement for particles above 1 mm. However, for small particles the model predicts a much higher conversion than the experimental data. Presently, there are large uncertainties connected with the experiments, leading to difficulties in drawing final conclusions based on this comparison.

4.0 CFD Modelling of biomass PF flame and comparison with measuring data

Presently work is in progress on making a comparison of measurements and CFD modelling of a 30MWth pulverized fuel biomass flame [Enclosures 5 and 6]. Measurements was conducted on a swirl stabilized biodust flame and the measuring data have previously been presented in a PhD thesis [3]. Water cooled probes were used to make a mapping of the near quarl flame area by inserting probes through the burner central tube and a side port. Also video and IR imaging of the flame was conducted. The local in flame measurements included gas concentrations (CO, CH₄, CO₂, NOx and PAH), temperature and LDA based axial and tangential velocities. Furthermore local particles samples were extracted and analyzed.

A RANS CFD modeling of the 30MWth swirl stabilized flame was successfully performed by use of FLUENT. The burner geometry and input parameters as air flows, particle size distribution, and kinetic data for devolatilisation and char combustion was specified. The applied computational domain included the burner and a box volume in the furnace chamber that enclosed the flame. The simulation provided detailed output data on local velocities, gas composition, temperature and particle conversion. Figure 7 provides an example of the obtained simulation data in the form of a temperature map of the near burner area. Maximum temperatures is experienced in the quarl area at positions where recirculated flue gas, fuel particles and secondary air is mixed.
This work have presently not been finished, so a complete conclusion cannot be provided, but some main results can be summarized. The simulations was able to capture the main features of the flame reasonably well including the rotating velocity field and the gas composition measurements. For the biomass particle devolatilisation kinetics a 0D model [6] was used, which was developed for isothermal modeling of wood particles. By comparison of measured and modelled temperature and gas species concentrations, it was seen that the flame ignition point was captured well. Gas phase velocities were found to qualitatively fit the measurements; however, an exact math was not obtained. A high degree of flame asymmetry has been observed from both flame measurements and the CFD simulation. This was caused by the gravitational pull on the fuel particles resulting in an asymmetric release of volatiles, and consequently asymmetric features of the flame was also observed at some distance from the quarl.

Both the flame measuring campaign and the CFD wood flame modelling have been very demanding tasks, but the results point towards that biomass flame CFD modelling can successfully provide realistic information on PF biomass flame behavior.

5.0 Review of biomass particle combustion at PF boiler conditions

Two studies regarding wood conversion were conducted in the CHEC program in parallel to this project, and was funded by several other sources (see enclosure 3 and 4). However, in the two studies biomass devolatilisation and char combustion was investigated, so a short summery of the main results of the two studies will be provided here.
Wood particle devolatilization experiments in a single particle combustor were done with 8 different wood types using particles with a diameter of 3 or 4 millimeters at temperatures from 1200 to 1450°C and with oxygen contents of 0 and 4.4 vol%. The influence of changes in moisture content, wood type and particle density on devolatilisation time was investigated. A 1D model was developed that accounts for internal and external heat transfer, water evaporation and devolatilisation kinetics. The model was compared with a broad range of experimental data and generally was observed a good agreement with the experimental data, and an example of this can be seen on figure 8. It was observed that devolatilisation time increases linearly with particle density and that wood type seems only to have a minor influence. When there was accounted for particle density and water content one set of kinetic expressions and heat transfer parameters could be used to model devolatilisation times of all the different wood types. Sensitivity analysis showed that biomass particle devolatilisation time at PF conditions is sensitive to particle size, moisture content, gas temperature and particle density, and insensitive to char yield.

There have, as seen in this report, been developed two 1D devolatilisation models. The model described in section 2 [model by Leth-Espensen et al. seen in appendix 2] covers a broader range of aspect ratios and was validated against particles with a broader size range (dp= 0.08 – 9.5 mm). The model was based on a shrinking core concept to model water evaporation and devolatilisation. The model described in this section [model by Luo et al. seen in Enclosure 3] was only set up for spherical particles, and applies a direct solving of heat transfer and kinetic equations. This model was only verified with particles in the 3 to 4 mm range, but it was validated on a broad range of different wood types. The influence of changes in parameters as moisture content, wood density and temperature were similar for the two models.

![Figure 8. Comparison between experimental and model predictions of devolatilisation time for beech wood at different reactor temperatures and densities of 4 mm spherical particles [from enclosure 3].](image)

Furthermore based on the 1D model (Luo et al.) a simple equation that can predict devolatilisation time as a function of biomass particle density, size, gas temperature and moisture content was made. Experimental devolatilisation time data found in the literature could be predicted within ± 25% for particles (1-10 mm) under high temperature conditions (1000 - 1600°C).
In addition, a study on char combustion was conducted with development of a model and comparison with data from the single particle combustion reactor [Enclosure 4]. The focus of the study was on the effect of gasification reactions on biomass char conversion under pulverized fuel combustion conditions. Experiments of pine and beech wood char conversion were carried out in a single particle combustor using the conditions of 1473-1723 K, 0.0-10.5% O₂, and 25-42% H₂O. A comprehensive progressive char conversion model, including heterogeneous reactions (char oxidation and char gasification with CO₂ and H₂O), homogenous reactions (CO oxidation, water-gas shift reaction, and H₂ oxidation) in the particle boundary layer, particle shrinkage, and external and internal heat and mass transfer, was developed. The modelling results are in good agreement with both experimental char conversion time and particle size evolution in the presence of oxygen, while some deviations are found for the gasification experiments. The modelling results show that the char oxidation is limited by mass transfer, while the char gasification is controlled by both mass transfer and gasification kinetics at the investigated conditions. A sensitivity analysis shows that the CO oxidation in the boundary layer and the gasification kinetics have a significant effect on the char conversion time, while the water-gas shift reaction and H₂ oxidation have only a small influence. Analysis of the sensitive of different parameters on the char conversion process under typical pulverized biomass combustion conditions (4% O₂, 13% CO₂, 13% H₂O), shows that the char gasification reactions contribute significantly to char conversion, especially for millimeter-sized biomass char particles at high temperatures.

Figure 9. The computed and experimental char conversion time of the pine and beech wood char particles under different conditions: pine wood char particles (3.2 – 3.3 mm) at the low temperatures: 1494/1483/1484 K, (a) and high temperatures: 1630/1722/1702 K, (b), and beech wood char particles at low temperatures: 1494/1483/1484 K, (c) high temperatures: 1630/1722/1702 K (d) [From enclosure 4].

In Figure 9 is shown a comparison between calculated and measured char conversion times and reasonably good agreements between model and measurements is obtained. The main difference between the model inputs for the two wood types is that the gasification kinetics rate for beech wood char is larger than for pine char. It shall also be remarked that the beech wood has a higher K content than the pinewood. As it is anticipated the model and the experiments shows that increased temperature, increased oxygen concentration and decreased char density leads to decreased char conversion times. It was observed, that if the gasification reactions and
the heterogeneous reactions in the boundary layer was not included in the model, then the modeled char conversion times were much larger than the experimentally determined char conversion times. This clearly shows that the conversion of biomass chars under PF conditions is not only controlled by the oxidation but also strongly accelerated by the gasification reactions. Model calculations predict that at typical biomass combustion conditions (4% O₂, 13% CO₂, 13% H₂O), the H₂O and CO₂ gasification reactions contribute to more than 50% of the char conversion at high temperatures (>1473 K) for both 3.2 mm pine and beech wood char particles. The char conversion is dominated by char oxidation for small particles (100 µm), while char gasification reactions become important for large particles (millimeter-sized).

A yet unpublished experimental study, which is in progress at CHEC, the char conversion of a very broad range of different biomass types is investigated at both oxidation and gasification conditions. There have been observed large differences in some of the wood samples gasification and oxidation conversion times. It may to some degree be that the alkali metals catalyze gasification kinetics, but other biomass properties may also be important. The conducted studies have provided data such that char yield and devolatilisation times can be reasonably predicted by modelling if biomass properties (size, density, K content) and local conditions are known, while further studies are needed before char conversion time can be predicted based on the biomass properties.

A short review study on biomass conversion in PF boilers have been conducted [Appendix 4A] based on the laboratory and modelling studies documented in this report, as well as some inputs from the literature. It was a main objective to put the obtained fundamental data into a broader perspective, and to investigate which biomass fuel properties that probably have the largest influence on flame behavior and fuel burnout in power plant PF biomass boilers.

On biomass PF boilers the combustion of the relatively large wood particles have been handled by making some modifications of the mill and the burners. However, the boilers sometimes experiences problems related to the wood pellet fuel, which is not easily understood based on the standard fuel analysis often conducted on the received pellets. Occasionally appears problems with poor burnout (high loss of ignition of bottom or fly ash) or problems with obtaining adequate flame ignition, such that the swirl-stabilized flames are lifted from the near quarl area. The review study provided information on particle properties that influences char yield, ignition, devolatilisation time and char combustion in wood PF boilers. The wood fuel properties related to devolatilisation mainly influence ignition and flame properties, while char conversion properties have a large influence on burnout. Some quite simple considerations on particles conversion can be done. Typically for high temperatures and large particles (as is the case for PF wood firing) kinetics is fast and transport phenomena’s have a controlling influence. In such a regime increased density or increased particle size will lead to both increased devolatilisation and char conversion time.

The wood pellets on PF plant is milled just before the pellets are transported with the primary air to the burners [13]. While milling mainly disintegrate the wood pellets into the original size some extra reduction of the particle sizes also often takes place in the mills. This implies that differences in milling propensity of different wood types may influence the wood combustion in the boiler.

The devolatilisation is controlled by external and internal heat transfer as well as by intrinsic pyrolysis kinetics. Most studies on devolatilisation at PF conditions (temperatures above 1000°C) have been done using particles larger or equal to 3mm [11, Enclosure 3] or smaller than 0.3 mm [7 - 10, and 12]. For the larger particles, no fragmentation was observed during devolatilisation and only a small shrinkage of approximately 20% was observed. For the smaller particles, that experienced higher heating rates, larger transformation of the particles
were observed [9, 12]. For wood particles with low alkali content, a complete melting of the particles during the devolatilisation process can be observed, and spherical char particles are formed. For particles with a higher alkali content less melting is observed, and some fragmentation seems to appear, however the degree of fragmentation has not been quantified.

The 1D model [Enclosure 3] that was developed of the devolatilisation conversion process do include heat transfer and kinetics, and was applied to conduct a few calculations on PF wood particle devolatilisation times. Calculated devolatilisation times are shown in Table 1. For the smaller particles, devolatilisation is so fast that this will contributes well to the flame ignition in the burner quarl area. Larger particles have much longer devolatilisation times, meaning that probably a significant fraction of smaller particles is needed to obtain a stable flame.

Table 1. Devolatilisation time as a function of temperature, density and water content calculated with the program developed by H. Luo et al. [From appendix 4 based enclosure 3].

<table>
<thead>
<tr>
<th>Case</th>
<th>Particle size, mm / Devolatilisation time, s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1 mm</td>
</tr>
<tr>
<td>Temp. °C</td>
<td>Density, g/cm³</td>
</tr>
<tr>
<td>1200</td>
<td>0.4</td>
</tr>
<tr>
<td>1500</td>
<td>0.4</td>
</tr>
<tr>
<td>1200</td>
<td>0.9</td>
</tr>
<tr>
<td>1200</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Ignition in wood dust flames is not investigated much. In some of our studies, we have seen that as soon some volatiles are released they immediately ignites in the high temperature environment of the applied reactors. This could lead to the conclusion, that wood flame ignition is very dependent on the initial release of volatiles. Calculations on the first 1% volatile release done by the model of H. Luo et al. [Enclosure 3] shows that for particles less than 0.1 mm it takes only a few milliseconds to obtain initial volatiles release. An increase in size or wood water content can significantly delay this initial release.

The combustion of the gas phase volatiles is relatively fast, while the char conversion is typically the most time consuming process and therefore also responsible for carbon left in the bottom and fly ash. Several studies on char yield have been conducted [9, 10, 12], and it is observed that particle size (and the derived heating rate) final temperature and wood alkali content plays a major role for the char yield. It is observed that the char yields are generally low at PF boiler conditions (always below 7 wt %), and this explains why relatively large wood particles (up to 2 mm) can be applied on PF boilers, and a fine burn out still can be obtained. It is also seen that an increased wood density or wood alkali content leads to an increased char yield.

The conversion of mm size char particles happens by direct oxidation, and by reaction with H₂O and CO₂ leading to a local formation of H₂ and CO, that is oxidized in the boundary layer. The char conversion process is therefore influenced by the transport of gaseous species, intrinsic reactivity and heat transfer [Enclosure 4]. As previously stated, large variations in biomass conversion time have been observed for different wood types, and that seems to be mainly related to differences in intrinsic kinetics towards CO₂ and H₂O. The kinetics can to some degree be related to the alkali content of the char, but other unknown parameters may also be important.
6.0 Conclusions

The project ‘Improved bio-CFD simulations’ have included activities on development of biomass particle devolatilisation models, performing drop tube devolatilisation experiments with particles from 0.6 to 1.5 mm, performing a comparison of inflame measurements and CFD modelling of a 30 MWth wood bio-dust flame and conducting a short review of the industrial implications of wood particle conversion studies.

The main conclusions regarding biomass devolatilisation in PF boilers, char yield, char combustion and use of CFD to simulate bio-dust flames are summarized below.

Devolatilisation

- A 1D model of wood particle devolatilisation conversion at PF conditions have been developed that covers particles sizes of \( dp = 0.08 - 9.5 \) mm and aspect ratios of \( AR = 1 - 8 \).
- A 0D wood devolatilisation model that is simple to apply in CFD modelling is developed based on the 1D-model results. The 0D model covers particles in the range \( dp = 0.08 \) to \( 3 \) mm.
- Very limited experimental data exist on wood conversion of particles from 0.2 to 3 mm at PF conditions. Some drop tube devolatilisation experiments with particles from 0.6 to 1.75 mm was performed, and the results was compared with the 0D model. A reasonable agreement was found between model and experimental data for particles above 1 mm. For smaller particles there was observed particle fragmentation induced by the devolatilisation process, and the model predicted higher conversions than observed by the measurements.

Char yield

- An equation is developed that can predict char yield from biomass devolatilisation at PF conditions based on an input of heating rate (calculated based on size and temperature), fuel alkali content and final exposure temperature.
- Generally are observed char yields bellow 7 wt% for wood devolatilisation at PF conditions

Char conversion

- An experimental and modeling study on char conversion have shown that heterogeneous gasification with \( CO_2 \) and \( H_2O \) plays an important role besides the direct \( O_2 \) oxidation. The wood char particle combustion model successfully predicted the char conversion of pine and beech wood, as well as the influence of temperature, oxygen content and char density.
- The conducted studies have provided data such that char yield and devolatilisation times can be reasonably predicted by modelling if biomass properties (size, density, K content) and local conditions are known, while further studies are needed before char conversion time can be predicted based on the biomass properties.

CFD use of the models

- In the project, some work on wood flame CFD modelling and a comparison of flame measurements and CFD modelling of a 30MWth pulverized fuel biomass flame was performed. Both the flame measuring campaign and the CFD wood flame modelling have been very demanding tasks, however the results point towards that biomass flame CFD modelling can successfully provide realistic information on PF biomass flame behavior.
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List of references