CFD-based modeling of kraft char beds – part 2: a study on the effects of droplet size and bed shape on bed processes

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ABSTRACT: This is the second of two papers. The first paper presented the char bed burning model used in this work. In this paper, the effects of liquor droplet size and bed shape on kraft char bed processes and lower furnace combustion are studied using a computational fluid dynamics (CFD)-based furnace model. The simulations show that droplet size affects not only the amount of in-flight conversion and the amount of combustible material reaching the bed, but also to what degree char carbon conversion in the char bed is due to direct oxidation or gasification. Droplet size also affects char bed burning indirectly through bed shape. Char bed shape affects the degree to which combustion air jets impinge on the bed surface, increasing carbon conversion by direct oxidation. In addition, changes in bed shape over time affect char bed processes. The results suggest that when a char bed starts to grow, the local carbon input to the bed could increase with bed height. In addition, carbon conversion decreases in locations of air jet impingement if the bed shape is not maintained.

Application: The CFD-based model for studying kraft char bed burning might help engineers and mills to better understand the lower furnace processes and optimize recovery boiler operations.

The recovery of pulping chemicals and energy contained in black liquor is a complex combustion process. Increased knowledge of char bed burning phenomena is important for better understanding the lower furnace combustion processes.

Computational fluid dynamics (CFD)-based modeling is a tool for studying kraft recovery furnace processes [1-12]. In simulations of black liquor combustion, the main sub-models describe droplet conversion, gas phase combustion, and char bed conversion. The char bed model is important in simulations of lower furnace combustion. The char bed shape is thought to affect char bed burning and lower furnace combustion processes, but its role is not fully understood. In this work, the effects of liquor droplet size and bed shape on kraft char bed processes and lower furnace combustion are investigated using CFD simulations.

BLACK LIQUOR COMBUSTION MODEL

The Åbo Akademi furnace model consists of application-specific sub-models for describing black liquor and bubbling fluidized bed combustion [10-13]. The black liquor combustion model includes description of black liquor droplet, gas phase, and char bed combustion.

Black liquor droplet combustion is described by a simplified model using results from single droplet experiments [10]. The model includes descriptions of drying, devolatilization, char combustion, and smelt bead formation. Liquor-dependent swelling of the droplets during combustion is considered. The droplet model is coupled with the gas phase, where combustion is described using a four-step methane reaction scheme [14].

The char bed model also is coupled with the droplet model and the gas phase. The description of the chemical bed processes is based on the principles of the stand-alone steady-state model of Frederick and Hupa [15]. Bergroth et al. [11] modified the original model and implemented it into the CFD environment. The model uses local mass and energy balances on the bed surface to calculate carbon conversion in the bed resulting from reactions with oxygen, carbon dioxide, water vapor, and sulfate. In addition, the bed temperature and a net carbon accumulation are calculated. Net carbon accumulation is calculated as the difference between carbon arriving with the droplets and carbon conversion [11].

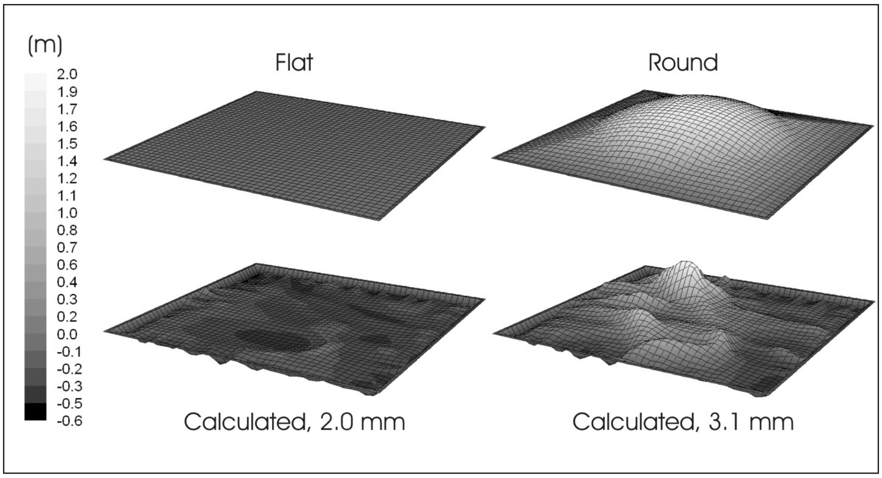
The shape of the simulated bed can be either presumed or calculated based on net carbon accumulation. The net carbon accumulation can be positive or negative, and thus, the bed can grow or deplete locally. The bed shape calculation is started from an initial shape, which is updated stepwise based on net carbon accumulation. For each new bed shape, combustion in the furnace (droplets, gas phase, and char bed) is recalculated and the new net carbon accumulation is used for the next change in shape. The change in bed shape during one step is relatively small (5-10 cm). The change in bed shape is associated with a time step, and as the process is repeated, the bed shape is calculated as function of time [12].

SIMULATION

The black liquor combustion model was used to simulate a 3150 tons dry solids/day recovery boiler. The process conditions for simulation input were well known, apart from the droplet size distribution in the liquor spray.

Process data

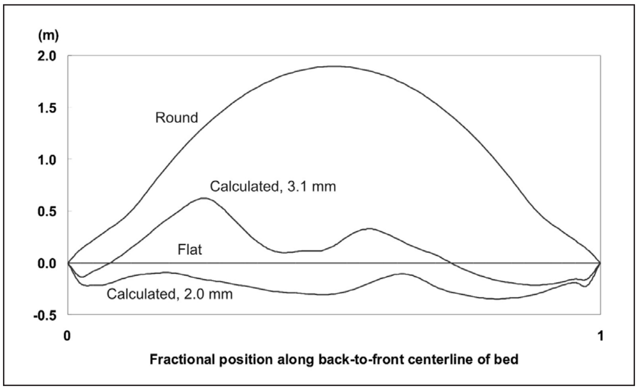
Process data relevant for set-up of the simulations included flow and distribution of combustion air, flow of black liquor, and number, location, and tilt of liquor guns. In addition, we carried out standard fuel analysis and determined the swelling properties and single droplet burning behavior of the black liquor. Based on these data, the amount and species of volatiles and amount of char carbon in the black liquor were determined [10]. Combustible carbon in black liquor was split 50:50 into volatile carbon and char carbon, respectively. The droplet size distribution in the black liquor spray was not measured; instead, it was assumed as described below.



1. Bed shapes used in simulations.

Simulation cases

Six simulation cases are included. Two average droplet sizes for the black liquor spray and four different bed shapes were used. For a Rosin-Rammler distribution function with spread parameter 2.9, the average droplet sizes were set to 2.0 mm or 3.1 mm. **Figures 1** and **2** show the bed shapes used in simulations. Two presumed bed shapes were used: flat and round. These represent shapes that could be imposed if the actual bed shape is unknown or if the bed shape is not calculated. The droplet sizes and presumed bed shapes were combined into four simulation cases. In addition, two simulation cases with calculated bed shapes were included. The calculated bed shapes are those after 30 min when starting from the flat bed and using an average droplet size of 2.0 mm or 3.1 mm. Using droplet size 2.0 mm resulted in bed depletion, whereas droplet size 3.1 mm resulted in bed growth. The actual recovery boiler usually is operated with a relatively flat bed [7], but during a special operational mode a mound grew and was depleted in a cyclic manner. In previous work [12], the calculated bed shape after 30 min using droplet size 3.1 mm corresponded well with that in the high-mound situation.



2. Height profiles of beds along the back-to-front centerline. In the beds shown in Fig. 1, the centerline goes from the 10 o'clock position to the 4 o'clock position.

RESULTS AND DISCUSSION

Material input to the bed

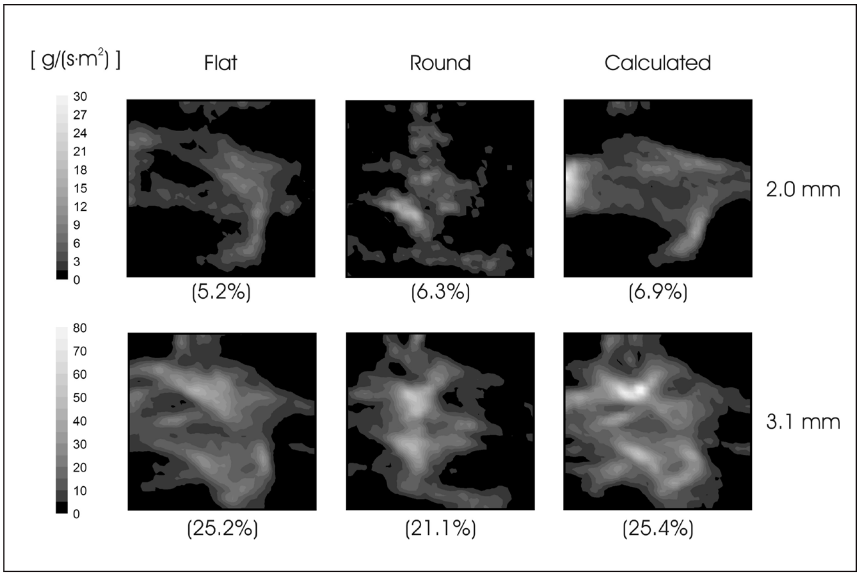
The average droplet size had a considerable effect on the amount of combustible material reaching the bed (**Table I**). With the smaller droplet size, more in-flight combustion takes place and only 5%-7% of the char carbon in the liquor feed reaches the bed; as opposed to 21%-25 % for the larger droplet

	Flat		Round		Calculated	
	2.0 mm	3.1 mm	2.0 mm	3.1 mm	2.0 mm	3.1 mm
In-flight conversion	66%	43%	69%	43%	69%	36%
To walls	29%	32%	25%	36%	24%	39%
To bed	5%	25%	6%	21%	7%	25%
Converted in bed	22%	25%	24%	23%	24%	24%

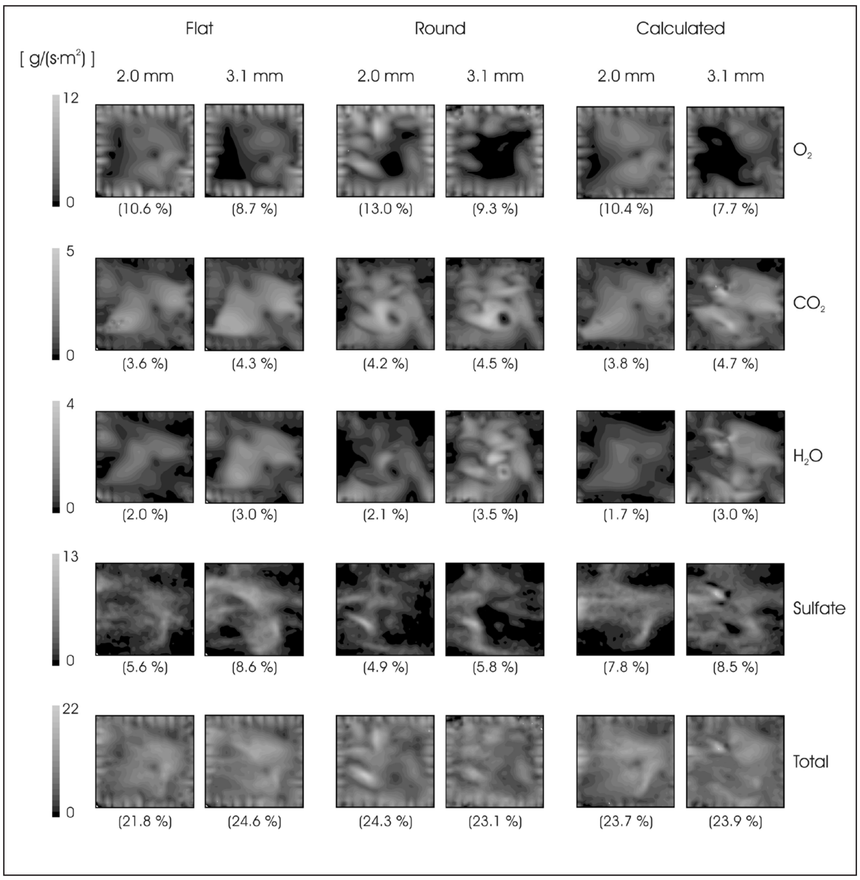
I. Fate of char carbon in simulated cases given as percent of total char carbon in the black liquor feed.

size. The maximum local carbon input also is higher when the bigger droplet size is used (**Fig. 3**).

The bed shape also affected carbon input to the bed (Fig. 3). With a higher bed, the material input is concentrated more toward the center of the bed. This is seen when using droplet size 3.1 mm and comparing the flat bed and the round bed. The center of the round bed is the highest location of that bed. When using droplet size 3.1 mm in the calculated bed, the material input is highest in the location of the highest mound, but input also is high in the other locations where the bed has grown. In general, because of the bed shape, the gas flow patterns above the beds are different; which affects droplet trajectories, in-flight combustion, and ultimately material input. When the bed height increases, the time for in-flight conversion of droplets is less and, as a result, material input to the bed increases. In addition, the simulations using the flat and the calculated bed shapes describe char bed processes at different moments in time. The char bed processes of the flat bed lead to the processes of the calculated beds, when given sufficient time. Thus, for material input, change in bed shape is associated with a feedback mechanism – when the bed shape changes, the material input also changes. When using droplet size 3.1 mm, material input increases locally with bed height. When using droplet size 2.0 mm, a difference in material input to the bed can be seen when the bed shape changes with time.



3. Carbon input to the char bed. Local carbon input contours are shown and overall carbon input is given in parentheses as percent of total char carbon in the black liquor feed.



4. Char bed burning in simulated cases. Local carbon conversion contours in the char bed are shown and overall carbon conversions are given in parentheses as percent of total char carbon in the black liquor feed.

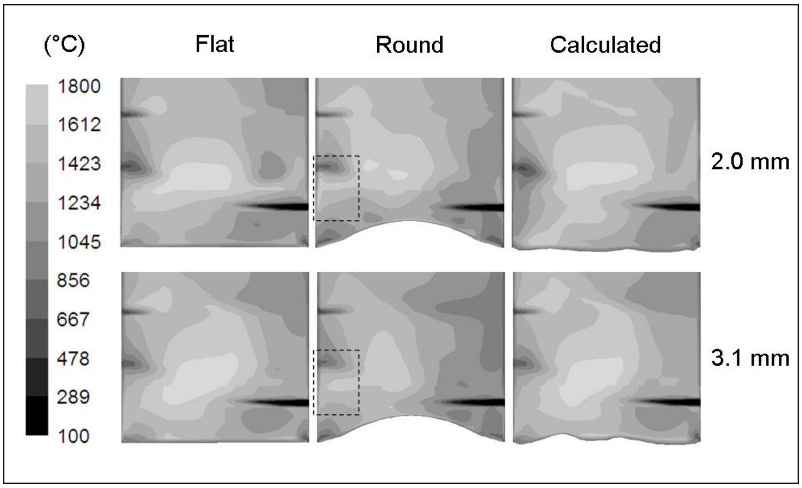
Char bed burning

Char bed burning was affected by droplet size (**Fig. 4**). With bigger droplets, in-flight conversion is less complete (Table I) and more volatile matter reaches the bed. More of the oxygen in the lower furnace combustion air is consumed in combustion of the volatiles and less is available for char bed carbon conversion. Increased droplet size decreases carbon conversion by oxygen by 18%-26% overall. However, the decrease is compensated for by an increase in carbon conversion by carbon dioxide and water vapor. This effect is seen especially toward the center of the bed. The compensation occurs to a high degree because char carbon conversion by the gas phase reactants was mass transfer-limited in all simulation cases. If the reactivity of the gasification reactions was lower, these reactions would compensate for the decrease in conversion by oxygen to a lesser extent.

With bigger droplets, more sulfate reaches the bed and carbon conversion by the sulfate reduction reaction increases. However, the full complexity of sulfate transport to the bed is not considered in the current version of the model; only the amount directly reaching the bed is included and sloughing from the walls is excluded. Thus, the sulfate in droplets initially hitting a wall does not contribute to char-carbon oxidation in the bed. In addition, the sulfate reduction degree in droplets is not tracked in-flight; instead, we use a constant value of 50%.

Char bed burning (Fig. 4) also was affected by bed shape. When using the round bed, the combustion air jets impinge on the bed surface and carbon conversion by oxygen is increased as compared with the flat bed. This is seen for the primary air jets around the perimeter of the bed and for the secondary air jets toward the center of the bed. The increased local carbon conversion by the secondary air jets is seen especially well when using droplet size 2.0 mm (Fig. 4). The increase in carbon conversion by oxygen overall in the bed is greater when using droplet size 2.0 mm (23%) as compared with using droplet size 3.1 mm (7%). However, in these simulations, the bed shape was presumed, meaning that the bed shape is fixed and independent of the predicted combustion processes. It also means that such a bed shape would not necessarily be formed during the operation of the boiler. When the flat bed shape is presumed, it more closely resembles the one usually present in an actual boiler [7]. The predicted char bed burning using the round bed describes the first seconds or minutes after the bed shape was first reached, and then liquor spraying and combustion air delivery were set according to the simulated conditions. Bed shape calculation was not carried out by starting from the round bed, but the overall carbon input versus conversion of the round bed (Table I) suggests that the bed shape is not stable if using the simulated operational conditions and that the bed would be depleted. As a result, the bed would tend toward a flatter shape. Such behavior would be in line with results from actual boilers, where liquor temperature can be changed to affect droplet size, and the amount of lower furnace combustion air can be changed to control char bed material input and conversion and, as a result, bed size.

Assuming the bed shape would change toward a flatter one, the high carbon conversion by oxygen in the round bed would decrease as result of depletion of the bed. The bed depletion would occur at a higher rate when using droplet size 2.0 mm versus droplet size 3.1 mm. A change in conversion by oxygen due to change in bed shape is seen when comparing the presumed bed shapes and the calculated ones. The calculated bed shapes have the common feature that the bed height around the perimeter is lower compared with that in the presumed bed shapes. Carbon conversion by oxygen is lower in these regions of the calculated beds as compared with beds with a presumed shape, and the differences are the result of changes in the bed shape. Carbon conversion by oxygen decreases as the bed burns away close to the primary air jets. In the simulations, the decrease in conversion is the result of a decrease in gas velocity above the bed. For actual char beds, the angle in which the primary air jets flow toward the char surface could affect burning; air jets impinging on the bed surface could result in higher mass transfer rates than predicted currently by the model. At the moment, the gas flow is assumed to approach the char bed parallel to its surface and the increase in mass transfer in locations of impingement is due to higher gas velocity only. In addition, char could be physically removed from the bed and become re-entrained in the gas flow.



5. Temperature contours in the lower furnace in simulated cases. The contours are along the back-to-front centerline. Dashed boxes indicate the location of increased temperature close to the furnace back wall when using the round bed.

Lower furnace combustion

Figure 5 shows temperature contours in the lower furnace. Peak temperatures are found at slightly higher elevations in the lower furnace when using droplet size 2.0 mm versus droplet size 3.1 mm. Although the effect of the change in droplet size in these simulations was minor, additional simulations using still larger droplets confirmed the general trend that smaller droplet size resulted in peak temperatures at higher elevations in the furnace, whereas larger droplets resulted in peak temperatures at lower elevations. This behavior is a consequence of differences in droplet trajectories resulting from droplet size, i.e., where the different sized droplets fly inside the furnace and where they burn. The lower furnace temperature profiles also were somewhat affected by bed shape; especially when using the round bed. Of the beds used, the round bed is most different in shape (Fig. 2), and the two calculated bed shapes resemble the flat bed more than the round bed. When using the round bed, the position of peak temperature is moved toward the back wall of the furnace. In Fig. 5, the location of increased temperature toward the back wall is indicated by dashed boxes. The predicted heat flux to the back wall is higher when using the round bed as compared with the other cases. The result could have some implications when considering the use of CFD as an engineering tool for troubleshooting or assisting in the design of a boiler, for example. Because the round bed is least representative of the bed shape typically present in the boiler, the predictions using the round bed should be considered least representative of the long-term conditions in the boiler. Although the actual bed shape of the simulated boiler is known, this is not necessarily always the case. Imposing a presumed bed shape that is not representative of the simulated conditions could contribute to a decrease in prediction accuracy.

SUMMARY AND CONCLUSIONS

We used a CFD-based furnace model to study the effects of droplet size and char bed shape on char bed processes and lower furnace combustion. The model was applied in a simulation of a 3150 tons dry solids/day black liquor recovery boiler.

The simulation results showed that droplet size and bed shape both influence the lower furnace combustion processes. The simulations confirm what is known from actual recovery boiler operations:

1) Droplet size – with liquor spraying as the operational parameter – has a considerable effect on the amount of combustible material transported to the lower furnace and the char bed. A bigger droplet size results in more material reaching the lower furnace, which in turn can contribute to bed growth.
2) Bed shape affects bed burning. With a higher bed, combustion air jets impinge on the bed surface, increasing burning by oxygen in those locations.

The simulations also give new insight into the details of how the studied parameters affect char bed processes and lower furnace combustion. With a bigger droplet size, the increased amount of combustible material and moisture reaching the lower furnace result in a decrease in oxygen concentration and an increase in carbon dioxide and water vapor concentrations above the bed. Although carbon conversion by oxygen is decreased, the decrease is compensated for by an increase in conversion by the gasification reactions. The degree to which this compensation takes place depends on the reactivity of char carbon. Assuming the oxygen-carbon reactivity remains unchanged and the gasification reaction reactivity varies, two extreme situations can be described:

1) With very low gasification reactivity, a decrease in oxygen concentration above the bed results in a direct decrease in overall carbon conversion.
2) With very high gasification reactivity, a decrease in oxygen concentration and an increase in carbon dioxide and water vapor concentrations does not result in a substantial, if any, decrease in overall carbon conversion by gas phase reactants.

A key consideration is the overall oxygen-to-combustibles balance in the lower furnace. A sufficient amount of lower furnace combustion air would tend to increase temperatures and provide oxygen for both gas phase combustion and char bed burning.

The simulations showed that changes in bed shape can affect bed processes over time. The results suggest that when a char bed starts to grow, the local carbon input to the bed could increase with bed height. In addition, carbon conversion in locations of air jet impingement decreases if the bed shape is not maintained. Thus, with sufficient time, the effects of droplet size and bed shape are not isolated; instead the lower furnace processes are coupled and affect each other. Although bed shape does affect bed burning, droplet size is the parameter that can be used to control the bed shape and size.

For CFD-based modeling, the results suggest that the bed shape is important. For increased accuracy, the presumed bed shape used in simulation of an existing boiler should match that of the real bed. In addition, when carrying out studies on the effect of operational parameters on furnace processes, the effect on bed shape also should be considered, and if or how the bed shape then affects the other furnace processes. Calculation of the bed shape offers an advantage over a presumed bed shape when studying the details of char bed burning over relatively long periods during which the bed shape is changing, or when studying lower furnace combustion process interactions affected by bed shape. **TJ**

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INSIGHTS FROM THE AUTHORS

The complex kraft char bed processes are not yet fully understood and thus are challenging and interesting research topics. Mathematical modeling and especially use of computational fluid dynamics (CFD) can aid in understanding the combustion processes and give valuable insights for both recovery boiler manufacturers and operators.

This research is a continuation of modeling work carried out at our research group and is extending currently available sub-models for predicting kraft char beds processes in the 3D computational environment.

The most challenging aspect of the research was implementation of the char bed sub-model into the CFD software for full 3D recovery boiler simulations. Validation is a key challenge to be addressed.

Among the more interesting findings from this study was the complexity of char bed processes; especially the interconnection between char bed shape and other char bed processes.

Ultimately, 3D dynamic mathematical models help engineers and mills to better understand the lower furnace processes and optimize the operation. The next step is model validation against observations from real boilers.

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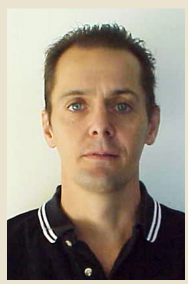

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