

Comprehensive model of alkali-salt deposition in recovery boilers

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ABSTRACT: Algorithms for alkali-salt deposition have been implemented into a comprehensive model for recovery boilers. The model includes (a) mechanisms for particle formation and chemistry, (b) particle deposition and adhesion, and (c) deposit thermal properties. These algorithms are fully coupled with models for turbulent flow, black liquor combustion, and heat transfer in the boiler. Model predictions for particle deposition in the convection pass are presented for a Babcock & Wilcox recovery boiler. This work is part of an ongoing project sponsored by the U.S. Department of Energy to demonstrate an improved ability to anticipate ash behavior with changes in fuel composition, operating conditions, and boiler design.

Application: Engineers and designers can use this model to understand problems with fouling and plugging and can help determine how to gain improvements in recovery boiler operations and design.

Deposit formation in recovery boilers is a major cause of boiler plugging and lost productivity. Inorganic material is generated in the furnace, becomes entrained by the combustion gases as particles and vapors, and is deposited on boiler surfaces. Heat transfer in boilers depends largely on the overall quantity, composition, and thermal properties of the inorganic material. Deposit formation in the convection pass represents one of the major limitations of the boiler both in operation and in design.

The mechanisms of deposit formation and the development of deposit properties are qualitatively understood for many fuels. For black liquor, ash deposition rates and properties were quantitatively measured in laboratory and *in situ* experiments [1-3]. Full-scale measurements have characterized particle size at various locations in the convection pass of the recovery boiler [4-6]. These measurements have established the presence of intermediate-size particles (ISP) that are larger than fume particles (aerosol condensates) and smaller than carryover particles (spray residues). Several research groups are now studying the mechanisms of ISP formation and the impact that ISPs have on boiler fouling. A previous modeling study that focused on aerosol dynamics and fume deposition in recovery boilers [7] was limited to a one-dimensional description of the convection pass and did not take ISPs into account.

In this paper, we present model predictions for a commercial boiler to demonstrate that new algorithms for deposit growth and deposit properties in a three-dimensional model of a recovery boiler

have improved our ability to predict fouling behavior.

MODEL DESCRIPTION

The comprehensive recovery boiler model (COMO-PR) of Babcock & Wilcox is designed to describe black liquor combustion in a recovery boiler, heat transfer, and steady, three-dimensional, turbulent flow. The model predicts:

- Combustion of black liquor spray and char deposits on the furnace walls and char bed
- Release of sodium, sulfur, potassium, and chlorine
- Quantity and composition of inorganic material (including carryover, ISP, and submicron fume) leaving the furnace
- Distribution of gas velocity, temperature, and chemical composition in the furnace and convection pass
- Distribution of convection and radiation heat transfer to the furnace walls and convection surfaces (which are the tube banks).

These modeling capabilities were previously described and demonstrated [8-11].

Convection pass surfaces

The furnace enclosure, superheater, generating bank, economizer, and cavities between tube banks are accurately represented in the model. Tube banks are simulated as a porous medium with properties to account for draft loss and heat absorption. The distribution of deposits and the local properties of the tube bank are represented within the resolution of

the computational mesh. Tube bank geometry (tube diameter, spacing, and arrangement) and local conditions (velocity, temperature, gas composition, particle size and composition, and deposit properties) are considered in the calculation of source terms for fluid momentum, turbulence, radiation, energy, particles, and chemical species.

Heat transfer and pressure drop in the tube banks

Heat transfer in the furnace and convection pass is solved with an equation for conservation of fluid enthalpy, where the fluid is a mixture of gases and fine particles (or fume and ISP). Fluid temperature is determined from thermodynamic relationships of enthalpy expressed as a function of temperature and chemical composition. Heat transfer is considered to take place by radiation and convection to the deposit surface and by conduction to the steam and water inside the tubes. Deposit temperatures and heat fluxes are evaluated from an energy balance at the deposit surface.

Radiation heat transfer is calculated with the discrete ordinates method [12]. Tube banks are treated as a participating medium that absorbs, emits, and scatters radiation like suspended particles. Radiation properties are calculated by assuming tubes are circular cylinders that act as independent scattering sources at the large particle limit, with tube diameter much larger than the wavelength of incident radiation [13]. Under these assumptions, the properties for radiation absorption and scattering can be expressed as a function of the tube diameter, spacing, and deposit emissivity.

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In the model, convection heat transfer coefficients are calculated from correlations for cross-flow over tube banks [14] based on local Reynolds number, tube diameter, tube spacing, and tube arrangement. Conduction heat transfer to the steam and water inside the tubes is assumed to be one dimensional in the radial direction. An overall heat conduction coefficient is calculated based on the thermal conductivity and corresponding thickness of each layer representing the gas-side deposit, tube wall, and steam-side deposit.

A body force is included in the momentum equations, which is equivalent to the pressure drop across the tube banks. A correlation for pressure drop across in-line tube banks [15] is applied in the direction perpendicular to the tubes. The pressure drop in the parallel direction is neglected.

Gas-entrained inorganic material

A detailed black liquor combustion model is used to predict the quantity and composition of inorganic material leaving the furnace [9, 10]. The distribution of gas-entrained inorganic material in the convection pass is modeled by solving conservation equations for the gas and for the three particulate classes of carryover, ISP, and fume.

Carryover particles ($> 100 \mu\text{m}$) are modeled by solving equations for conservation of mass, momentum, energy, and chemical composition ($\text{C}_{(g)}$, Na^+ , K^+ , Cl^- , CO_3^{2-} , SO_4^{2-} , and S^{2-}) in a Lagrangian reference frame. Particle position, velocity, mass, temperature, composition, and physical properties are calculated along each trajectory, representing a group of particles with the same attributes. A stochastic particle dispersion model accounts for the effects of turbulence on particle motion. Particle impaction and sticking are modeled by removing particles from the group, while other particles are considered to rebound and continue along the original trajectory. The trajectory is extinguished when all of the particles are depleted. Several thousand trajectories are calculated to determine the distribution of particles and deposition rates in the convection pass.

Intermediate-size particles ($1\text{--}100 \mu\text{m}$) are modeled by solving equations for conservation of mass and chemical components ($\text{C}_{(g)}$, Na^+ , K^+ , Cl^- , CO_3^{2-} , SO_4^{2-} , and

S^{2-}) in a Eulerian reference frame. These particles are assumed to be of a uniform initial diameter of $30 \mu\text{m}$. Intermediate-size particles are small enough that they are assumed to follow the gas flow, and the rate of turbulent diffusion for ISP is considered equivalent to that of the gas.

Fume particles ($0.1\text{--}1 \mu\text{m}$) are modeled by solving equations for conservation of mass and chemical species. The local quantity and composition of fume is determined from multiphase chemical equilibrium between sodium, potassium, and chlorine vapors, and gas-phase combustion products. Aerosol dynamics for nucleation, condensation, and agglomeration of fume are neglected. Fume particles are assumed to be of uniform diameter ($1 \mu\text{m}$). These particles are small enough that they can be assumed to follow the gas flow, with the rate of turbulent diffusion set as equivalent to that of the gas.

Deposition in the tube banks

The tendency for molten particles to deposit on a tube surface is characterized in terms of capture efficiency, η , which is equal to the product of the collision and the adhesion efficiencies: $\eta = \eta_c \times \eta_a$. The collision efficiency, η_c , is defined as the fraction of particles passing through the projected area of the target that actually collide with the target. The adhesion efficiency, η_a , is defined as the fraction of particles that stick to the surface after they collide.

Figure 1 shows the collision efficiency plotted against particle diameters typical for particle deposition on a generating bank tube in a recovery boiler. Collision efficiencies are calculated with algorithms for inertial impaction, eddy impaction, and thermophoresis.

Inertial impaction. Large particles (carryover and ISP) deposit on a tube in cross-flow by the mechanism of inertial impaction. In theory, large particles deviate from gas streamlines and may collide with the surface as the flow accelerates around the tube. Inertial impaction is calculated based on correlations for collision efficiency for flow past a circular cylinder [16].

Under ideal conditions, the direction of flow approaching a rectangular-pitch tube bank is normal to tube rows, and inertial impaction does not extend beyond the first row of tubes. Particles impact the first tube, and a "buffer zone"

of particle-free fluid is created downstream that shields other in-line tubes. Inertial impaction is calculated based on correlations for collision efficiency for flow past a row of tubes [17].

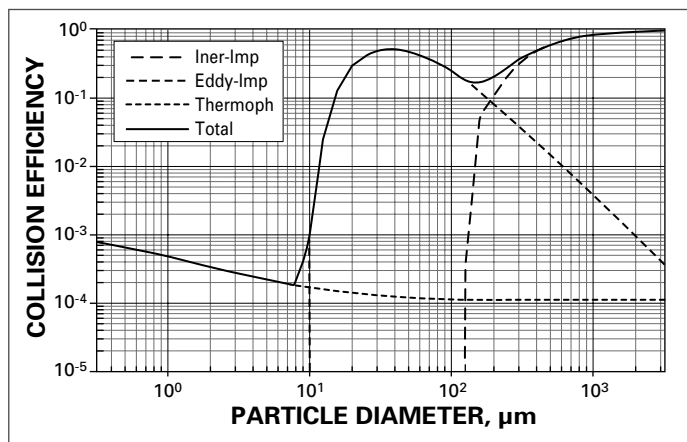
When the direction of flow approaches the bank at an oblique angle, the first row of tubes does not completely shield other in-line tubes, and inertial impaction can extend beyond the first row. Therefore, a method was developed to apply the algorithms for inertial impaction to tube banks in oblique cross-flow.

Collision efficiency for inertial impaction (Fig. 1) is zero below a critical diameter (or Stokes number), then it increases rapidly with diameter to a maximum of one, the theoretical upper limit. Therefore, carryover ($>100 \mu\text{m}$) can potentially have the highest deposition rate on the basis of the weight of deposits per unit weight of particles approaching a tube bank.

Eddy impaction. Eddy impaction plays an important role in the deposition of particles in turbulent channel flow. This mechanism is based on the theory that turbulent eddies impart momentum to particles in a direction that is normal to the main flow. In the vicinity of a surface, particles can attain enough momentum to cross the boundary layer and impact the surface.

For cross-flow over in-line tube banks, the flow lanes between in-line tubes act like channels. Particles that are not captured by inertial impaction on the first row of tubes are channeled into the flow lanes between tubes. These particles are transported by turbulent eddies in the direction normal to the main flow. They impact on a neighboring tube if they have enough momentum to penetrate the boundary layer around the tube. In the wakes behind tubes, vortices form and contribute to velocity fluctuations in the direction of transverse flow.

An algorithm for eddy impaction in tube banks was developed based on first principles of particle aerodynamics and on model predictions of turbulent velocity fluctuations within tube banks [18]. The collision efficiency of eddy impaction (Fig. 1) first increases with diameter as particles attain more momentum to cross the boundary layer and then decreases with diameter as eddies have diminishing influence on particle motion. The magnitude of the collision efficiency peak depends on the intensity of the turbulence.



1. Particle collision efficiency (typical).

Eddy impaction plays a significant role in carryover and ISP deposition. However, fundamental data are needed to validate model predictions of eddy impaction rates.

Thermophoresis. The mechanism of thermophoresis (or Soret diffusion) dominates for small particles that are driven across the boundary layer by Fick diffusion, augmented by a temperature gradient. Accurate methods for calculating thermophoretic deposition rates have been demonstrated [19], and these methods can be used to predict fume deposition in boilers.

Recent experimental data [1] have shown that (a) fume deposition does not appear to be controlled by thermophoresis, as widely assumed, and that (b) fume deposition rates are linear in time and are insensitive to changes in the temperature gradient near the surface. Therefore, surface renewal theory was proposed as a possible mechanism for describing the fume deposition rates found. However, this mechanism has been neglected in our model and will continue to be neglected until a meaningful correlation with laboratory data is developed.

Collision efficiencies for thermophoretic deposition (Fig. 1) gradually decrease with particle size. This mechanism is only important for fine particles (fume). At diameters greater than about 10 μm , the effect of thermophoresis is negligible compared with the effect of impaction rates.

Particle adhesion

Fundamental experiments of carryover deposition in an entrained flow reactor were conducted in Canada at the University of Toronto, and particle adhesion efficiency was correlated with particle size and liquid content [20]. These results were used to develop an algorithm for particle adhesion efficiency, which is shown in Fig. 2. Particle adhesion is zero at liquid fractions below a critical value, after which it increases to a

maximum value. The liquid fraction at the onset of sticking and the maximum adhesion efficiency both increase with particle size. The *sticky temperature* is defined as the temperature at which liquid content is 15%. This temperature is the point at which carryover with a nominal diameter of 200 μm begins to stick.

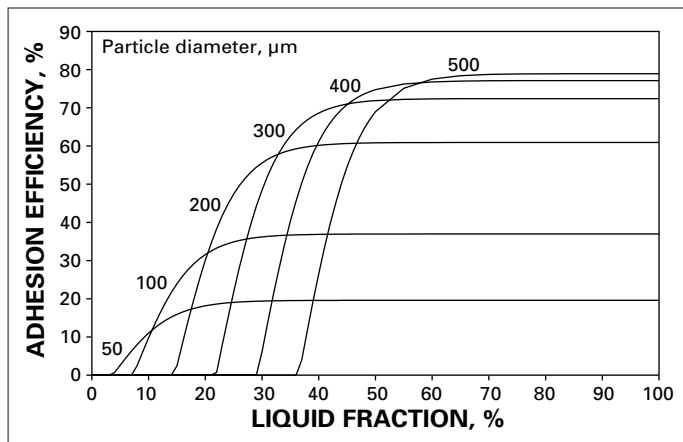
The predicted temperature and the composition of carryover and ISP were used to calculate the liquid content and adhesion efficiency of particles when they impact a surface. Liquid content was interpolated from data obtained from Åbo Akademi University (ÅAU) in Finland. These data were calculated on the basis of an advanced multi-component phase equilibrium model [21] over a range of temperatures and a matrix of carbonate, potassium, and chloride compositions.

The algorithm for particle adhesion was used only to describe particle impaction and rebound mechanisms. Fume deposition, which is governed by the mechanisms of particle diffusion, is assumed to have an adhesion efficiency of 100%.

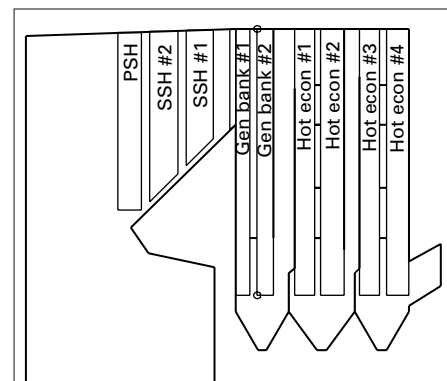
Deposit properties

In situ measurements of deposit emissivity and thermal conductivity have been reported [1, 2] and are characterized in terms of the size, porosity, and structure of deposit particles. A method for simulating dynamic deposit growth and properties was developed from these data. Particle deposition rates are integrated as a function of time. The effects of sintering [22] on linear shrinkage, porosity, and deposit properties are included in a dynamic model. However, time-dependent predictions of deposit growth and deposit properties have not been implemented in the comprehensive model at this time.

The distribution of deposits and the deposit properties can be represented in the comprehensive model within the



2. Particle adhesion efficiency.



3. Schematic of convection pass surfaces (PSH = primary superheater. SSH = secondary superheater.).

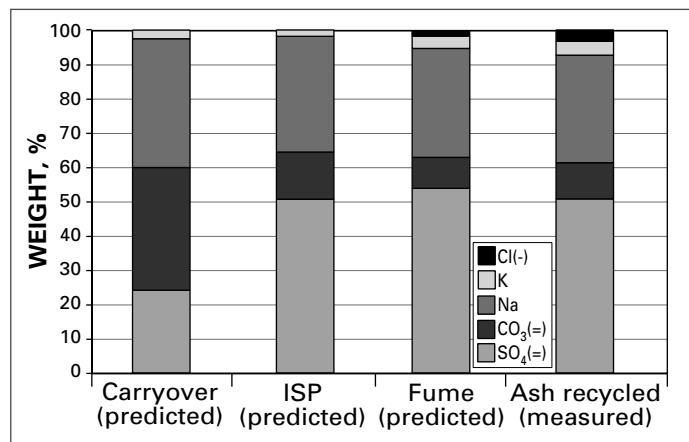
	$T_{0'}$ °C	$T_{15'}$ °C	$T_{70'}$ °C	$T_{100'}$ °C
Carry-over	754	781	803	807
ISP	810	816	831	835
Fume	563	653	783	805

1. Melting behavior of entrained particulate.

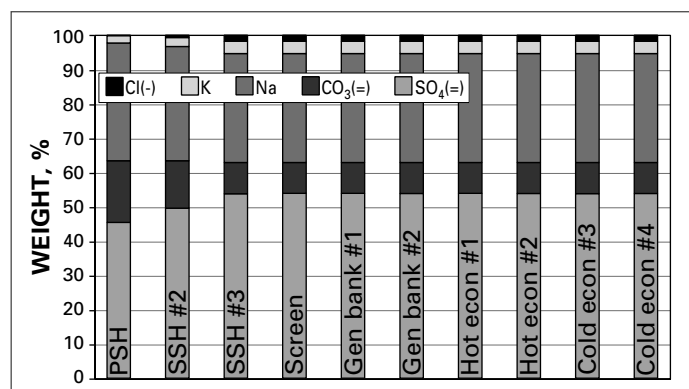
spatial resolution of the computational mesh. The typical size of a control volume in the computational mesh (~ 0.3 m) is too large to represent variations in deposit properties from tube to tube, around the circumference of a tube, or across the thickness of a deposit. Therefore, intrinsic properties of a deposit are represented in the model as mass- or area-weighted averages.

Correlations for emissivity of fume and molten ash deposits [10] are used for the furnace walls and tube banks. Deposit thermal conductance is currently specified for each surface, assuming that deposit thickness and thermal conductivity are fixed. These properties are used in energy balance equations to predict deposit surface temperatures and heat flux.

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4. Predicted particle composition.



6. Predicted deposit composition.

MODEL RESULTS

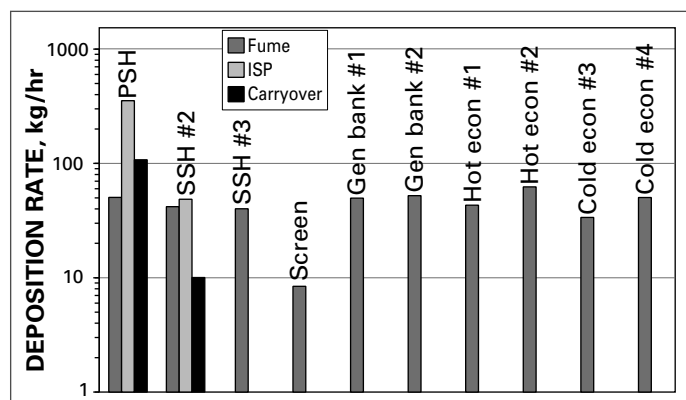
A recovery boiler that was experiencing problems with fouling and plugging of convection surfaces was used in this modeling study of deposit formation and properties. The boiler is a single-drum design supplied by B&W. Figure 3 shows the arrangement of the surface in the convection pass, including the primary superheater, the secondary superheater (SSH), the long-flow generating bank, and the long-flow economizers.

Process modeling results

The boiler was tested during stable operation over about an 8 h period. It burns a mixture of black liquor from several mills. The liquor has more chlorine and potassium in it than it should, which contributes to plugging problems. The gross heat input per plan area was 2.12 MW/m², which is below the average of 2.5–2.7 MW/m² for boilers of this size. Boiler operating conditions used during performance testing were summarized previously [10, 11].

The comprehensive model is useful for predicting process information which characterizes the boiler performance. Figure 4 shows the predicted compositions of carryover, ISP, and fume, and Table I gives the corresponding melting behavior. As Fig. 4 shows, the model predicts the composition of fume to be close to the measured composition of dust samples collected from the electrostatic precipitator (designated in the figure as "Ash Recycle").

Furthermore, the model predicted the quantities of entrained particulates to be 155 kg/h for carryover, 2691 kg/h for ISP, and 3301 kg/h for fume. This prediction for the quantity of fume is in



5. Predicted deposition rates.

good agreement with the measured ash recycle rate (3992 kg/h). The quantity predicted for ISP is large relative to the quantities predicted for fume and carryover, but this result is not unexpected based on ISP generation rates measured in laboratory experiments. The predicted carbonate content increases with particle size, and chloride content decreases with particle size, as expected. Predicted levels of potassium and chloride enrichment in the fume are also in good agreement with measurements.

Carryover and ISP particles are stripped of chlorine via chloride vaporization during combustion. The chloride vapor condenses as fume. Predicted levels of chlorine in the carryover and ISP may be low because the limitations of chloride diffusion within the particle were neglected and the condensation of chloride (and fume) on the surfaces of large particles was neglected.

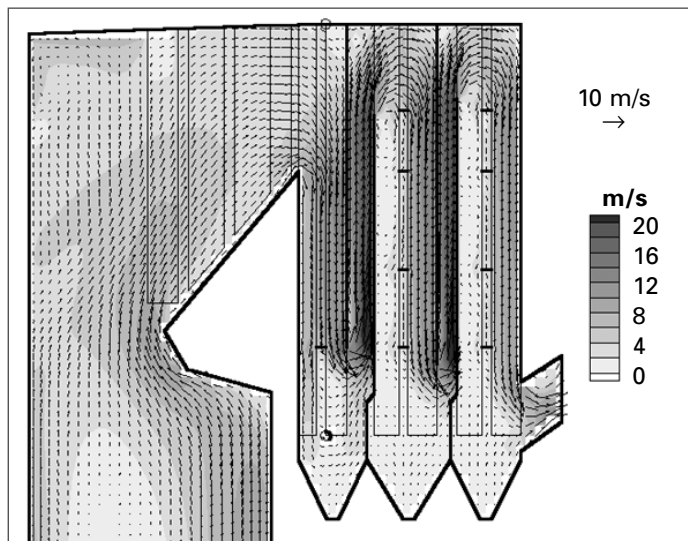
Figure 5 summarizes the predicted deposition rates at each bank of the convection pass. Carryover and ISP deposition is confined to the first and second bank of the superheater, where particles were still molten and the adhesion efficiency was greater than zero. These particles were predicted to solidify over a narrow range in temperature as a result of low chloride levels. If the model's predictions of high ISP concentrations are accurate, the deposition of ISP is greater than carryover. Fume deposition does not vary significantly from bank to bank.

The predicted deposit composition is shown in Fig. 6. Carbonate levels are higher in the superheater, where carryover and ISP are deposited. Downstream from the superheater, the chloride content is higher, and the deposit composition is equivalent to the fume composition.

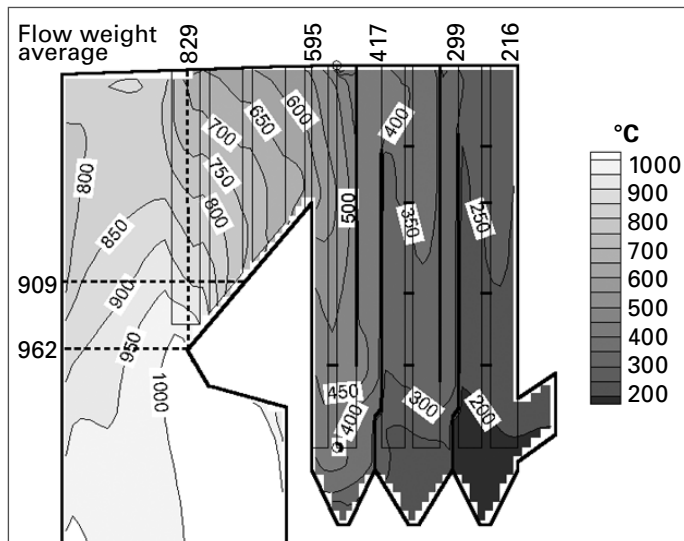
Detailed modeling results

Three-dimensional modeling results also provide detailed information needed to understand deposit growth and its impact on boiler performance. Figures 7–11 show modeling results in a two-dimensional plane through the center of the convection pass. As Fig. 7 shows, gas enters the superheater at an angle that is roughly parallel to the top of the nose arch, exposing the bottom of the primary superheater to high gas temperatures (Fig. 8), high carryover and ISP deposition rates (Fig. 9), high deposit temperatures (Fig. 10), and high heat flux (Fig. 11). Deposition by carryover and ISP particles does not extend past the gas temperature contour of about 750°C, because impacting particles do not stick after they solidify. Deposits on the primary superheater are partially molten, but most surfaces are below the radical deformation temperature (T_{r0}) at this reduced load (Fig. 10).

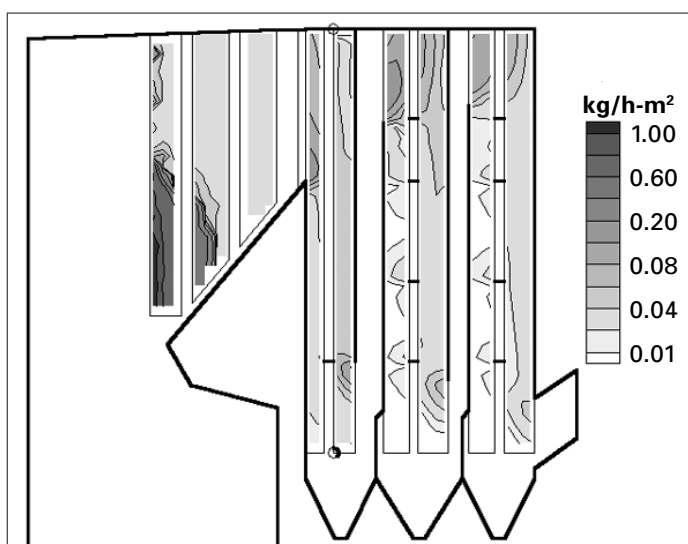
Gas enters the generating bank in cross-flow, then becomes parallel with tubes, and exits the bank in cross-flow (Fig. 7). The



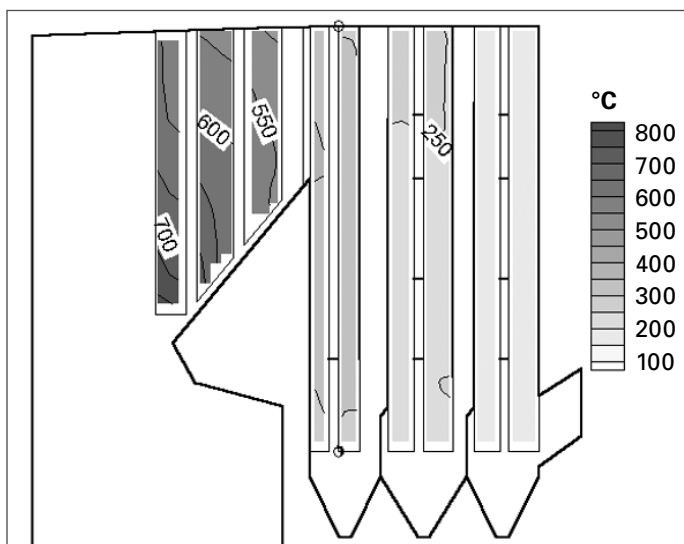
7. Gas velocity.



8. Gas temperature.



9. Total deposition rates.



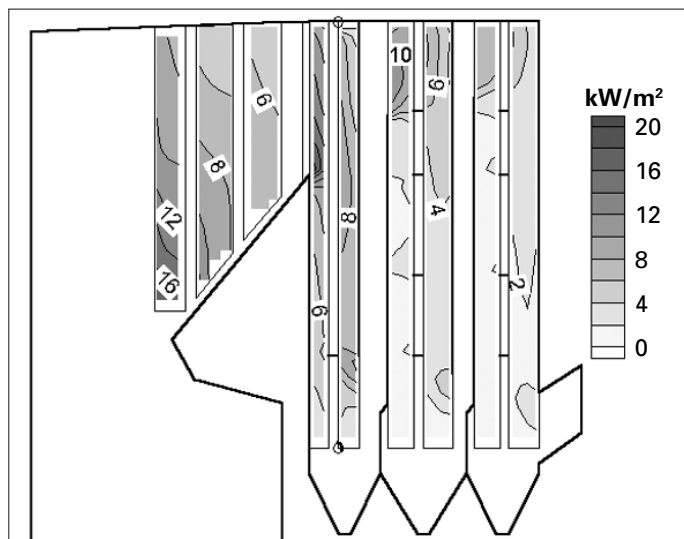
10. Deposit surface temperatures.

regions of cross-flow with the highest velocity correspond to regions with the highest fume deposition rates (Fig. 9). These regions have been observed to build up deposits rapidly and require more frequent sootblowing. The patterns of fume deposition are repeated in the hot and cold economizer banks. However, sootblowing is more effective in the economizer because the temperature is well below the sticky temperature and fume-sintering rates are low.

Side-to-side imbalances in velocity and temperature leaving the furnace cause more carryover deposition on the left-hand side of the boiler (not shown). These imbalances put an uneven heat load on the superheater and cause high temperatures and depositions of carryover and ISP to move closer to the generating bank on the left side. If sticky temperatures of carryover and ISP reach the tightly spaced tubes of the generating bank, then the growth of tenacious deposits may plug the boiler.

CONCLUSIONS

A model was successfully developed for predicting alkali salt deposition in the convection pass of a recovery boiler. Results from three-dimensional modeling provide detailed information that improves our understanding of deposit growth and its impact on boiler performance. Modeling can be used qualitatively to elucidate problems with fouling and plugging, leading



11. Total heat flux.

to more effective use of convection surfaces and sootblowing.

With greater validation, the model will be a useful engineering tool for anticipating ash behavior with changes in fuel com-

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position, operating conditions, and design. Further model development is planned and will include implementation of time-dependent behavior of deposit growth and property development. We also plan to further investigate ISP formation and concentrations in recovery boilers to determine the impact on fouling and plugging. **TJ**

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