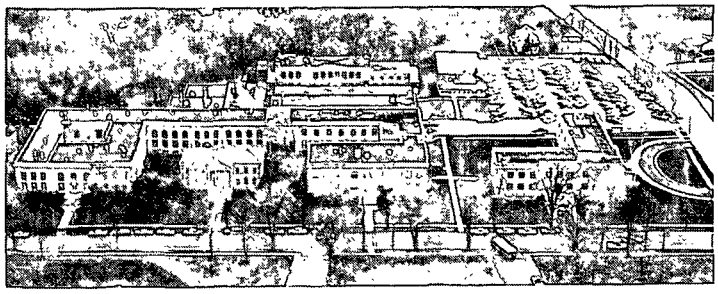

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A THREE-DIMENSIONAL MATHEMATICAL MODEL OF THE KRAFT RECOVERY FURNACE

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ABSTRACT

The paper describes the construction and preliminary results from a three-dimensional mathematical model of a kraft recovery furnace. The model is based on a computational fluid dynamics package (FLUENT) that is modified to incorporate in-flight black liquor particle burning and char bed burning. Simulations with this model can provide extraordinary insight into the nature of the combustion process in the recovery furnace. The model demonstrates that the main mode of burning in the furnace is particle burning. Carryover is shown to be not simply determined by liquor spray size but rather by a very complex relationship between drop size, gas flow patterns, and oxygen concentrations. Gas flow patterns are determined primarily by the air inlet geometry and conditions and are not greatly modified by liquor sprays and in-flight combustion. Bed shape, on the other hand, can have a marked effect on gas flow patterns. The model promises to be a powerful tool for acquiring a better understanding of recovery furnace operation and for examining alternative firing techniques and furnace design features.

INTRODUCTION

Although mathematical models of recovery furnaces have been used for many years for special purposes, they have severe limitations. A critical need is the ability to relate critical performance parameters (extent of carryover, gas temperatures, combustible and oxygen concentrations, bed growth or depletion, reduction efficiency, etc.) to the firing practice and furnace design. This can only be done with a three-dimensional model which can handle the complex gas flow patterns that exist in recovery furnaces. Previous models are essentially one-dimensional and are primarily directed toward material and energy balance information over different zones of the furnace. Empirical splitting fractions are used to force fit the model to experience. A few two-dimensional particle trajectory models exist, but these do not handle realistic flow fields. Within the past few years, independent efforts at The Institute of Paper Chemistry and at Tampere Technical University have produced realistic three-dimensional models of the kraft recovery furnace. This paper describes the construction of the IPC model, which we call FLUENT-RFM, and presents some of the results from the first few simulations performed with the model.

MODEL STRUCTURE

FLUENT-RFM is a fundamental three-dimensional model of the kraft recovery furnace that is based on a finite-volume solution of the governing equations for mass, momentum, energy, and species concentration for the gas phase. In-flight burning of liquor drop/particles and bed burning are included and affect the gas phase through source-sink terms. The model is constructed around a commercially available computational fluid dynamics code (FLUENT), with appropriate modifications to incorporate the critical features of kraft recovery furnaces.

Gas Phase

The gas flow velocities are found by a finite-volume solution of the mass, momentum, and energy conservation equations in three-dimensional geometry. The furnace volume in divided into a large number of cells (50,000 in our case) and the difference equations are solved numerically. The interaction between the liquor phase and the gas is handled through source/sink terms using the psi-cell approach. In the psi-cell (particle source in cell) approach, the gas phase conditions (velocity, pressure, enthalpy, and chemical composition) are treated as a continuum in a fixed coordinate system. The properties of the gas are then a function of position only. The properties of the liquor phase are described in a reference frame moving with the individual drop/particle and are determined at small discrete time steps as the particle passes through the gas phase. Trajectory equations for individual drops are written in a fixed reference frame and are coupled with state equations that describe the drop properties as a function of time. The drop/particles are able to exchange mass, momentum and energy with the gas phase through source and sink terms in the gas flow equations. The position of a drop/particle at any time, t, uniquely determines which cell it is in. The change in state properties become the source and sink terms and are added to the cell in which the drop/particle is in at time, t. The approach is illustrated in Figure 1. If the drop is drying as it passes through the cell,

the amount of water evaporated from the drop during that interval would be a mass source of water vapor to that cell, and the amount of heat absorbed by the drop would be an energy sink.

The gas phase properties of interest are the three velocity components, pressure, temperature, density, and species concentration. The gas species considered are oxygen, water vapor, carbon monoxide, carbon dioxide, fuel (pyrolysis gases), and inerts (nitrogen). Sulfur gases are not handled in the present state of the model. Temperature is determined from enthalpy balances using temperature dependent specific heats for each of the gas species. Gas density is determined using the ideal gas law. Turbulence is handled through effective gas properties determined from the k-epsilon model of turbulence. Radiation energy fluxes are determined from a six-flux radiation model, one flux in each of the positive and negative coordinate directions. Rates of chemical reactions between gases can be controlled by either a chemical reaction rate or by the degree of turbulent mixing. In practice, the rates were controlled by turbulent mixing.

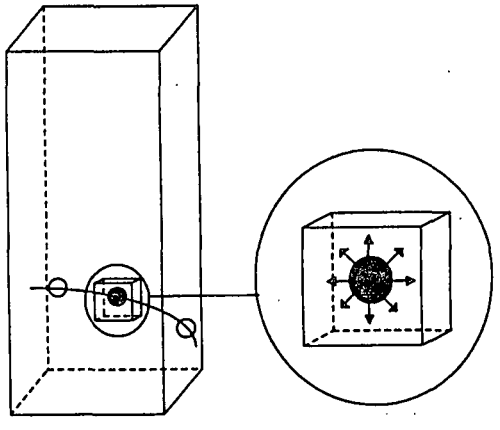

Figure 1. Illustration of PSI-cell approach.

Black Liquor Phase

The behavior of the black liquor phase was described by trajectory equations for the individual drop/particles and by a drop combustion model. The trajectory equation relates the change in particle momentum to the drag force exerted on the particle by the gas and to the force of gravity. The drag force is related to the square of the relative velocity between the particle and the gas, the particle cross-sectional area, the gas density and a drag coefficient. Standard correlations for spheres are used for the drag coefficients. At present, the number of drops used in a simulation is 10,000. Each drop represents an equal mass fraction of the spray and each drop has a unique initial position, velocity, and diameter. The diameter distribution was assumed to be log-normal. The initial speeds of all the drops were assumed to be the same, regardless of size or direction. Angular boundaries in the vertical and horizontal plane are set and the mass of the spray is assumed to be evenly distributed between the boundaries.

The combustion is modeled as four distinct stages; drying, volatiles burning, char burning and inorganic oxidation. Drying is treated as an external heat transfer controlled process. Some swelling of the drop during drying is allowed. Ignition signals the start of the volatiles burning stage. The solids content at which ignition occurs is a user-specified parameter. Volatile burning is handled by an empirical rate equation developed by Crane [1]. Swelling during volatile burning is handled by assuming the drop diameter increases linearly during the volatile burning period, reaching a maximum at the end of the period. The user specifies the maximum extent of swelling. Char burning is treated as an oxygen mass transfer limited process. A standard Sherwood number correlation for flow past a sphere is used to calculate the mass transfer coefficient. The volume of the char particle is allowed to decrease during char burning in a linear fashion with the mass of carbon remaining. At the end of the char burning period, the inorganic smelt drop is allowed to oxidize and convert sodium sulfide to sulfate. The rate of oxidation is treated as an oxygen mass transfer limited process. The user sets the maximum allowable mass increase, in effect setting the sulfidity and reduction state after char burning.

The species in the drop/particle are water, fuel, fixed carbon and ash (inorganic). The information on the liquor supplied by the user is summarized in Table I. Liquor density and diameter determine the initial mass of the drop. Solids content determines water, fraction volatiles determines fuel, fraction char carbon determines fixed carbon and the amount of smelt oxidation represents the fraction of sulfur that can be oxidized. Water is transferred to the gas phase during drying, fuel is transferred during volatiles burning, fixed carbon is converted to CO and CO_2 during char burning, and inorganics are allowed to oxidize after char burning is complete. The mass exchange terms and oxygen sinks that are calculated by FLUENT/RFM are shown in Figure 2.

Table I. User supplied parameters for liquor phase.

Composition	Burning Characteristics
Liquor density	Solids content at ignition
Solids content	Swelling during drying
Fraction volatiles	Swelling during volatiles burning
Fraction char carbon	
Amt. of smelt oxid.	$CO/(CO + CO_2)$ ratio

Spray Parameters

Initial diameter distribution
Vector velocity distribution

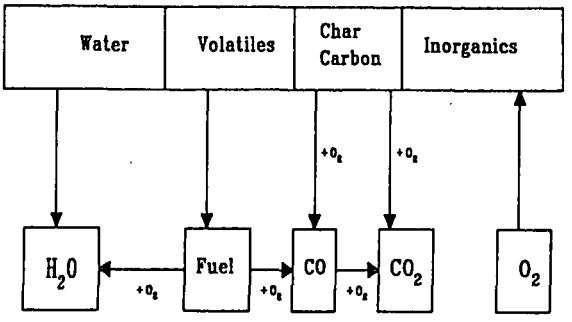

Figure 2. Mass exchange between liquor and gas phases.

Char Bed

The char bed is modeled using a special type of cell, the bed cell. Bed cells act like wall cells in that they act as a barrier to flow, but they differ in being able to exchange mass and energy with the gas phase (normal wall cells can only exchange energy). All of the bed behavior is assumed to occur at the interface between the bed and the gas phase. The bed is a sink for oxygen from the combustion air and from oxidized smelt drops landing on the bed and a source for CO and CO_2. The burnup of carbon by oxygen is assumed to occur through a sulfate-sulfide cycle. Oxygen reaching the bed is assumed to oxidize sulfide to sulfate and this rate is assumed to be controlled by the rate of oxygen mass transfer. Any sulfate present is allowed to react with carbon by a temperature dependent kinetic expression. This permits the state of reduction to be determined as a resultant of two competing rate processes. Gasification of the char carbon by reaction with CO_2 and H_2O is also allowed. Heats of reaction for the individual bed reactions are accounted for, and the bed is able to exchange heat with the gas phase above by radiation and convection. The temperature of each bed cell is determined by an enthalpy balance over the cell.

Bed cells do not operate at steady state as far as the carbon material balance is concerned. The temperature- and gas composition-dependent rate processes determine the rate at which char carbon is consumed on the bed. The rate at which carbon is supplied to any particular area of the bed (any particular bed cell) is determined by particle trajectories above the bed and the associated particle state variables. These do not normally balance on any given cell. The model simply keeps track of the rate of carbon accumulation or depletion in any given bed cell. The bed reactions per se only involve char carbon and inorganic. If the material landing on the bed is not fully dried or pyrolyzed, the residual water and/or fuel content is put directly into the neighboring gas cells.

The trajectories of some of the drop/particles may cause them to strike the wall. These are handled by assuming any liquor particle striking the wall sticks, dries, and partially pyrolyzes and then falls down to the char bed. For all material reaching the wall, all of its residual water and 1/2 of its residual fuel are transferred to the neighboring gas cells. The rest of the material is then directed to the char bed immediately below.

Overall Structure

The choice of FLUENT as the computational fluid dynamics code underlying the model was based on its versatility, applicability, and the availability of the source code for modification. Model development included writing original code for black liquor burning in flight and on the char bed, and modifying the base FLUENT code to provide for the five chemical species in the gas phase, revising the combustion model, and providing the source and sink terms needed to communicate with the bed and in-flight burning models. The overall structure of FLUENT/RFM is shown in Figure 3.

BASE CASE SIMULATION

Description

The first complete converged solution of the model was done for a generic recovery furnace referred to as the "base case". The furnace geometry is shown in Figure 4. The furnace is 10 meters by 10 meters by 30 meters high. The bull nose, located on the back wall, occupies about one-half of the furnace cross-section. There are three basic levels of air entry. Primary air is modeled as a slot extending the entire length on all four walls. The width of the slot is chosen so that the total primary air port opening matches typical values. Secondary air is located two meters above the primary air. A total of 36 secondary air ports are used, evenly spaced on all four walls. Tertiary air is located on the front and

back walls at two different elevations above the liquor gun openings. Nine ports are used on each wall and they are staggered and interlaced so that no tertiary nozzles are directly opposed to each other. The bottom row of tertiary nozzles is located 8.5 meters above the floor and the top row is 1.25 meters above the bottom row. Four liquor guns are used, located 6 meters above the floor at the midpoints on each wall. The bed shape is a truncated pyramid extended to a level just below the secondary air ports. A symmetry plane is used (only 1/2 of the furnace is actually modeled) in order to make the most effective use of the 50,000 nodes.

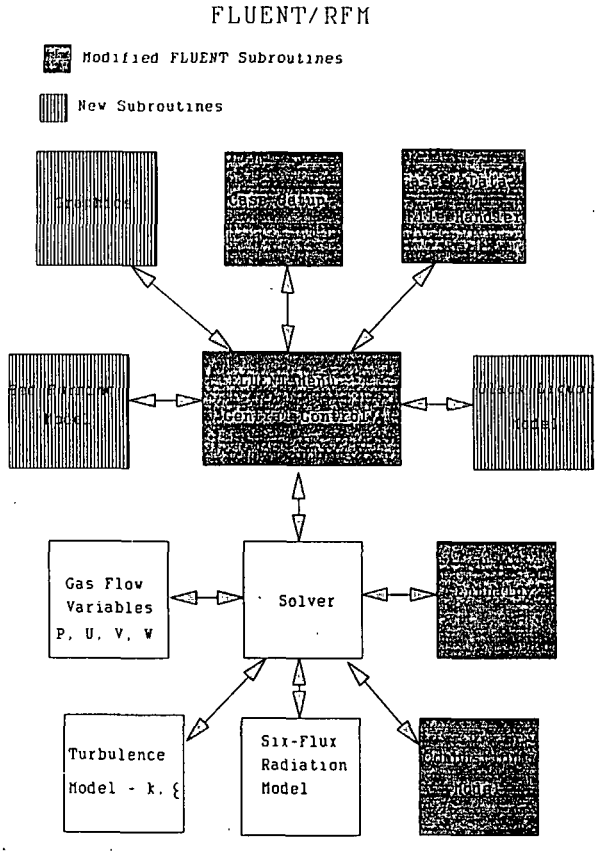

Figure 3. Structure of FLUENT/RFM.

The black liquor solids firing rate is 11.0 kg/m^2 min (2.25 lb/ft^2 min). The solids content is 65% and the high heating value is 6600 Btu/lb. The mean drop diameter was 2.5 mm. The total air rate is 86.2 kg/sec (about 10% excess air). The primary air is 45% of the total at an entrance velocity of 43 m/sec, secondary air is 34% of the total at 39 m/sec, and the tertiary air is 21% of the total at a velocity of 93 m/sec. The air temperature was 400 K.

Results

The model is capable of giving a great deal of information about the burning process in the furnace. At each node point the vector velocity, temperature and concentration of each species in the gas phase is found. Particle trajectories and state information is available. Thus carryover rates and bed char fluxes can be determined. In addition composite rates of drying, volatile burning, char burning, etc., as a function of position can be determined and displayed. Heat fluxes to the walls and to the char bed can be found. Average reduction rates are also calculatable.

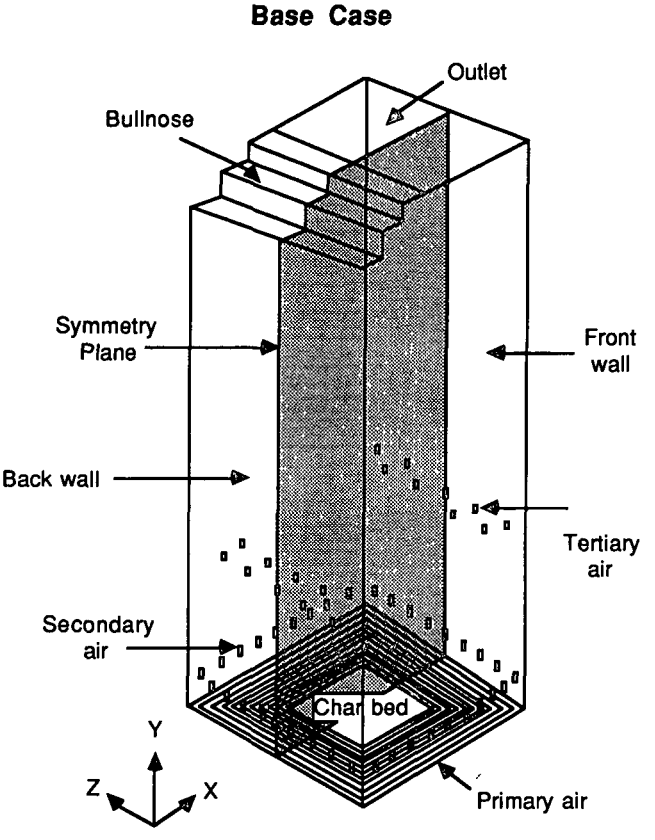

Figure 4. Base case geometry.

The gas flow paths determined by the model for the base case are complex but in general agreement with expectation. The dominant feature, illustrated in Figure 5, is a central core of high upward velocity. Around the perimeter, particularly in the corners, is a region of downflow. The core is disrupted by the tertiary air jets but reforms above the tertiary air level and persists past the bullnose and out of the furnace cavity. The core is formed by the convergence of the four wall primary and secondary air above the char bed. The role of the char bed in central core formation is shown in Figure 6.

Gas temperatures tend to be highest in the core, and the O_2 concentrations the lowest. Average gas temperatures as a function of height are shown in Figure 7. The general shape of the curve agrees with experience. The peak in tem-

perature occurs slightly above the surface of the char bed where large amounts of CO and pyrolysis gas are present and able to react with secondary air. Three dimensional distribution of temperature and gas concentrations is complex and strongly coupled to details of the gas flow pattern and particle trajectories.

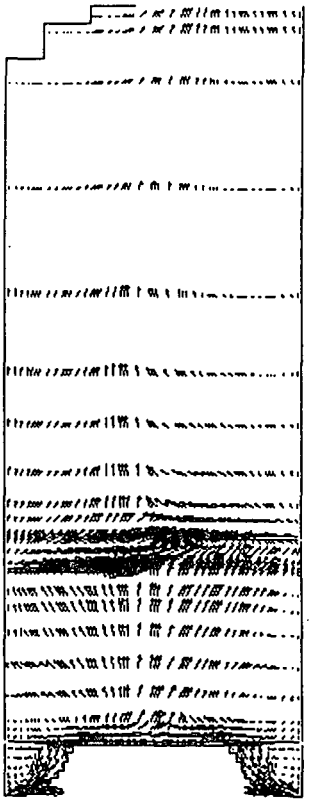

Figure 5. Gas flow pattern at center plane.

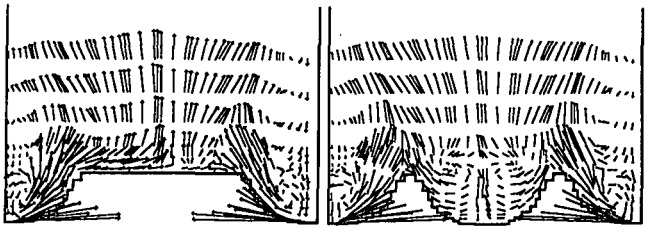

Figure 6. Effect of bed shape on gas flows.

Black liquor burning is highly complex and dependent on the details of flow patterns, gas temperatures and O_2 concentrations as well as initial drop size and velocity. Carryover of particles out of the furnace cavity, in particular, is highly interdependent on many variables. Color raster plots of the trajectories of drops with an initial diameter of 0.5 mm are very different for the nozzles on the front, back and side walls. Thus drop size and average gas velocity are not the only determinants to carryover.

Most of the material falling to the bed falls around the perimeter of the furnace. A map showing the flux distribution of carbon and inorganic landing on the bed is given in Figure 8. Part of the perimeter flux is due to wall drying and pyrolysis, but the nature of the gas flow pattern also tends to favor material striking the bed near the walls. The bed model also indicates that carbon gasification by reaction with CO_2 and H_2O is an important part of bed burning. Figure 9 shows bed burning data calculated from the model with and without the gasification reactions included. The addition of the gasification reactions converts the base case from one in which there is substantial buildup of carbon on the bed to one where there is a slight depletion of carbon.

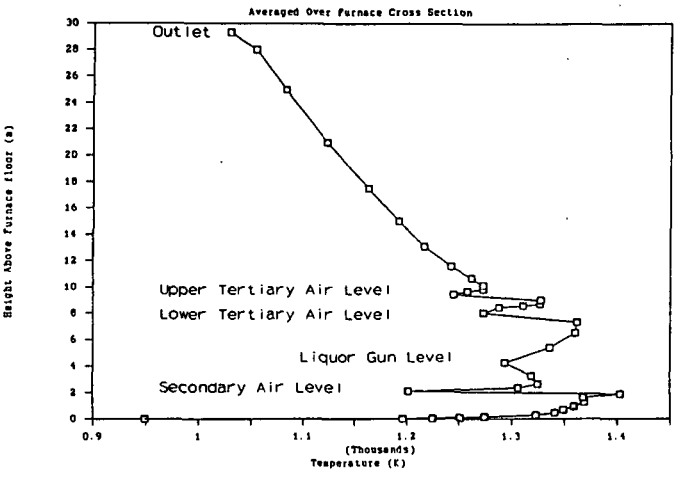

Figure 7. Temperature as a function of furnace height.

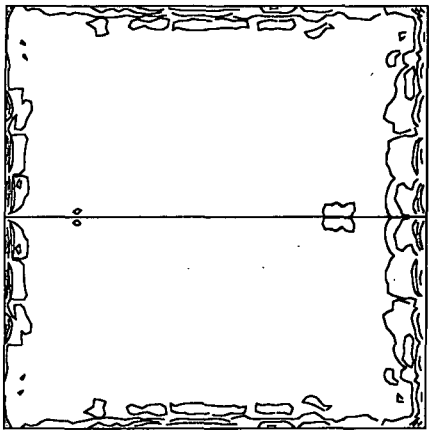

Figure 8. Map of carbon and inorganic flux to bed.

Process Insights

The model and the results of the base case simulation provide a great deal of insight into the processes occurring in recovery furnaces. The important role of in-flight burning is clearly evident. Burning of black liquor is primarily a process of drop/particles burning in

flight and not one of burning gases produced by pyrolysis and gasification of material delivered directly to the char bed. Oxygen is consumed wherever the particles are present, and the majority of that consumption takes place above the bed. There are limits on the amount of combustion which can take place on the char bed which are imposed by limitations on the ability to transfer oxidants (primarily oxygen) to the bed.

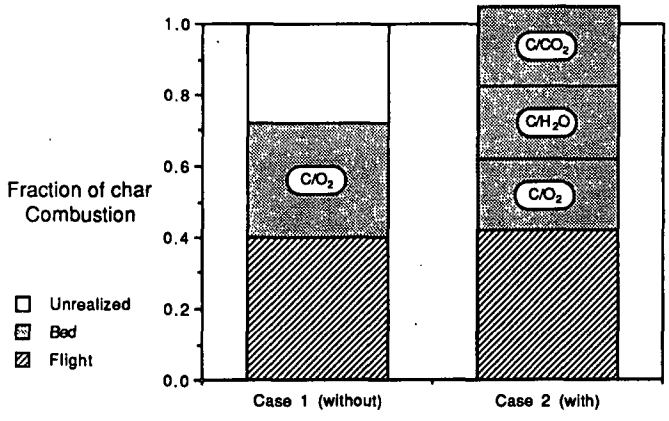

Figure 9. Comparison of char combustion without and with gasification reactions.

Carryover of material out of the furnace is very complex. There are two distinct modes of carryover, and the variables which control each mode are different. One type is carryover of dense smelt drops which are small enough that their terminal velocity is less than the upward velocity of the gas stream that they are caught up in. The key variables for this mode are drop size and gas velocity, and the temperature and composition of the gas has little effect. The second type is carryover of low density partially burned particles. Black liquor can swell greatly during volatiles release and burning, and the particle only gradually densifies again during char burning. Thus the rate and extent of char burning of in-flight particles is very important, since this controls the particle density and hence the ease of carryover. The extent of carryover of unburnt particles is very strongly influenced by oxygen concentrations in the vicinity of the particle, since the char burning rate is directly proportional to the oxygen concentration. This can override the influence of gas velocities and initial drop size.

The dual nature of carryover is clearly shown in Figure 10. The extent of carryover is not a monotonic function of initial drop diameter. Carry over is high for the smallest drops (the ones that carryover as smelt drops) and then drops off. However, at intermediate sizes the carryover amount again increases and forms a local maximum. This is due to the carryover of incompletely burned liquor particles. The smaller particles require shorter burning times and densify quicker and are not carried over as easily. The biggest particles have higher terminal velocities throughout their histories and get to the bed much more easily. The data on particle in-flight residence times given in Table 2 supports this interpretation. The coupling between the extent of inflight combustion and carryover is also evident in Figure 11 which shows the oscillatory approach to convergence as the number of iterations increased. Oscillations in inorganic carryover have greater amplitude and are directly in phase with oscillations in char combustion extent. It can be shown that these in turn were coupled with slight oscillations in the oxygen concentration in the core.

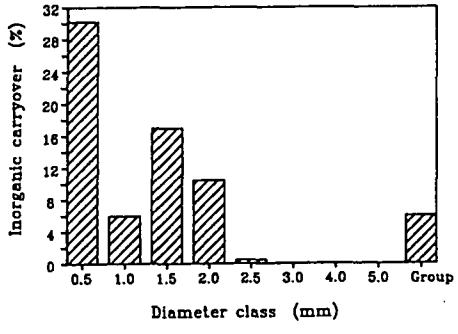

Figure 10. Inorganic carryover vs. initial drop diameter.

Table II. In-flight residence times of particles (in seconds).

	Initial Drop Diameter, mm								
	0.5	1.0	1.5	2.0	2.5	3.0	4.0	5.0	lognormal
	Particles Striking Bed								
Average	4.1	4.7	4.7	3.5	5.0	2.5	1.4	1.2	3.3
Max.	7.4	12.6	21.4	20.0	19.7	19.0	1.7	1.4	28.2
Min.	1.8	2.6	1.3	1.2	1.2	1.2	1.2	1.2	1.1
	Particles Carried Over								
Average	8.4	6.1	6.6	7.8	8.7	---	---	---	7.4
Max.	29.8	9.0	10.3	10.5	8.7	---	---	---	22.0
Min.	4.6	4.9	4.9	5.8	8.7	---	---	---	4.6

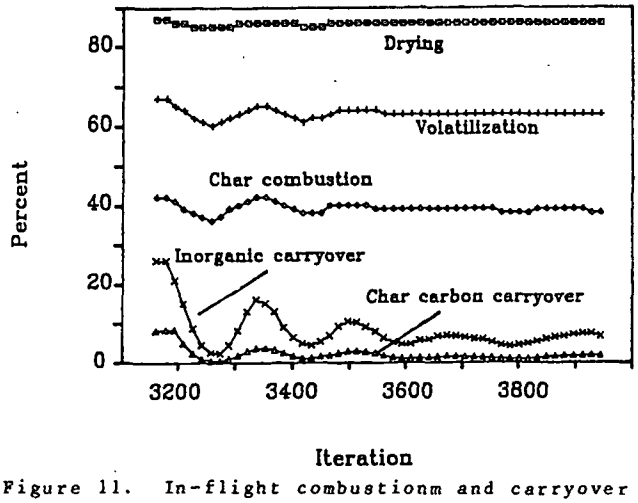

Figure 11. In-flight combustionm and carryover coupling.

The model results cast some doubt on the commonly held notion that more uniform spray size distributions will result in less carryover. It was shown, for example, that the same size drops behave completely differently when introduced on the front, back and side wall nozzles. There is clearly a small drop size cutoff, below which smelt drops have a high probability of being entrained. In addition, very large drops are likely to reach the bed in a wet state which would interfere greatly with bed burning rates. However, it is not clear that uniformity inside this range is beneficial. It is possibile that highly uniform sprays might cause the combustion process to be more unstable. Further simulations are needed to resolve this issue.

The gas flow patterns appear to be determined primarily by the geometry and conditions at which the air enters the furnace and only secondarily by the liquor sprays and the combustion process. The bed shape, however appears to exert a strong influence on gas flow patterns and the intensity of the central core. This suggests that questions about gas mixing and air jet penetration can be resolved by cold flow testing and by flow models which ignore the combustion process, provided the bed is handled properly. In a given furnace, control of the gas flow patterns would be pretty well set by the air distributions and pressures and not highly dependent on other aspects of the operation. There is an implication that some bed shapes are preferred to others and that this should be considered in selecting firing strategies and manipulating spray variables.

Breaking up the center core by momentum transfer may not be the primary function of the tertiary air. There is evidence in the base case simulation that the core was disrupted by the tertiary jets but then reformed above the tertiary elevation. Since particle burnout is a key factor in carryover, it is possible that the most crucial role of the tertiary air is to reinject oxygen into the central core to allow char carbon burnout.

Introducing gasification reactions into the char bed model had a very significant impact on bed burning rates and on the temperature and concentration distributions above the bed. Published data on the rates of char gasification by CO_2 and H_2O is very sparse and the expressions used in the model have a high degree of uncertainty. This is an area where data are urgently needed.

MODEL STATUS

A converged solution of a recovery furnace simulation using all of the features present in FLUENT/RFM has been obtained. The results are reasonable and consistent with experience. Behavior which is not in accordance with conventional wisdom is readily interpretable and provides new insight into what is truly happening inside recovery boilers.

Convergence is a major problem. Convergence requires a certain amount of operator interaction as it proceeds and some 3500 iterations, involving about 12 trillion mathematical operations, are needed to get a converged solution. About 3 months of CPU time were needed for the base case simulation on a MicroVAX II. The long time needed to obtain a solution has restricted the number of cases which have been run so far. A major effort is now underway to speed up the code and to access faster machines so as to reduce the time for solutions by a factor of 100.

Another limitation imposed by machine constraints and the long convergence times is the use of a plane of symmetry. At present we are only able to model furnace geometries that have side to side symmetry. This eliminates many cases of interest such as tangential tertiary air and side wall interlaced secondaries, since the gases do not flow across the symmetry plane. The means for overcoming this limitation are readily apparent and this is also a part of further developments.

The model as it currently exists does not include sodium and sulfur chemistry. Ultimately this needs to be part of a recovery furnace simulation model, since sulfur gas concentrations and dust loads are important operating parameters. S/Na chemistry is not included in the present model because the necessary rate equations for sulfur release and dust production have not yet been developed, and because these reactions have only a very minor effect on the basic combustion, flow and temperature data. Plans are underway to develop a model to handle sulfur and sodium chemistry that would use a converged solution without sulfur and sodium chemistry as a starting point.

The final issue is model validation. No attempt at modeling an actual recovery boiler operation and comparing the results with field data has been made as yet. In fact very few sensitivity tests of model parameters have been made to date because of the long convergence times. The model is based on fundamental principles and does display many of the features

qualitatively known to exist in recovery furnaces. It would be premature, however, to blindly use the model for simulating an actual furnace. Model validation with actual furnace data will be done over the next two years and this should greatly increase the reliability of model predictions.

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End