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**COMPUTATIONAL SIMULATIONS  
OF INDUSTRIAL FURNACES**

*by*

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## COMPUTATIONAL SIMULATIONS OF INDUSTRIAL FURNACES

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### ABSTRACT

This paper presents results from computer simulations for three different industrial furnaces. The furnaces include a gas fired ethylene process heater, a coal fired cyclone pre-combustor barrel for a power utility boiler and a cyclone copper smelter. The systems have been modeled using a CFD-based two phase, reacting flow model. The modeled systems are highly complex and thus model "validation" is typically in the form of agreement with qualitative, historical knowledge from plant personnel. Where available, comparisons with quantitative field data are included. Overall, the models are shown to have good agreement with qualitative trends and acceptable agreement with quantitative data.

### INTRODUCTION

There has been a dramatic increase in recent years in the use of comprehensive CFD based computational tools to model industrial processes within the Chemical, Metallurgical, and Power Generation Industries. For many in these industries, this has been a significant change in philosophy. Historically, these industries relied on cold-flow experimental scale models or 1-D zonal computational models to perform product/process R&D and to guide scaling of pilot or laboratory data for full size facilities. The motivations for the paradigm shift are varied: pressures for increased productivity; global expansion of markets; tighter pollution emission regulations; reducing the time to develop new products; and reducing the time to bring new processes/plants into full production.

Using a reliable computational model which provides full coupling of all relevant physical processes allows the engineer to determine sensitivities to design changes without relying on simplified empirical models that are often extrapolated beyond the conditions for which their validity has been proved. To properly model industrial systems requires computational tools that

properly describe the first-order physics and chemistry that drive the system. The model should have full mass, momentum and energy coupling between the gas and particles as well as full coupling between turbulent fluid flow, chemical reactions, radiative and convective heat transfer.

Reaction Engineering International (REI) uses and markets a suite of comprehensive CFD based computational tools that have been used to simulate reacting flow fields and heat transfer in a wide range of industrial process reactors, furnaces and boilers. Our computational tools represent over 20 years of continuous development by Dr. Philip J. Smith and co-workers [1-7]. The types of systems that can be modeled include: utility boilers, chemical process heaters, waste incinerators, metal processing systems and stack flares [1][2]. Our combustion simulation tools can be used to model reacting and non-reacting gas and particle flows, including gaseous diffusion flames, pulverized coal flames, liquid sprays, coal slurries, injected sorbents and other oxidation/reduction systems. Particular emphasis has been placed on simulating coal combustion, pollutant formation (fuel, thermal, and prompt NO<sub>x</sub>) and pollutant reduction (reburning, SNCR models). Our software tools have undergone extensive testing to determine their capabilities and limitations. The results of these studies have demonstrated that the models are capable of predicting qualitative information (trends), and in some cases quantitative information, to within sufficient accuracy to justify engineering design changes.

The intent of this paper is to demonstrate the types of real-world, operational problems in complex, industrial systems that can be addressed with CFD-based modeling tools. As such, the first section in this paper contains an overview of the CFD-based two phase, reacting flow model; modeling. Subsequent sections present results for modeling: a gas fired ethylene process heater, a coal fired cyclone barrel and a cyclone copper

smelter. References are provided for the interested reader that would like further details on the models and results described herein.

## TWO PHASE REACTING FLOW MODEL

The modeling of industrial scale combustion systems requires the integration of several complex phenomena. The gas-phase flow field itself is very challenging due to the need to accurately model turbulent, swirling flow. Modeling two-phase flow systems containing reacting particles adds more complications. Because the particles carry momentum, the particles must be tracked separately from the gas flow field. In addition, for reacting particles, while tracking the particles through the furnace the model must also compute the reactions that are occurring within the particles and the mass (volatiles) released by the particles. In industrial systems, the furnace temperatures can range from 300K to over 2000K. Thus radiation effects must be included. In general, the reactions that take place lead to extremely large heat release. The associated gas temperature and density changes have a significant effect on the flow field. Thus a tightly coupled solution algorithm is required.

The REI combustion models employ a combination of Eulerian and Lagrangian reference frames [1-7]. The flow field is assumed to be a steady-state, turbulent, reacting continuum field that can be described locally by general conservation equations. The governing equations for gas-phase fluid mechanics, heat transfer, thermal radiation and scalar transport are solved in an Eulerian framework. The governing equations for particle-phase mechanics are solved in a Lagrangian reference frame. The overall solution scheme is based on a particle-in-cell approach.

Gas properties are determined through local mixing calculations and are assumed to fluctuate randomly according to a statistical probability density function (PDF) which is characteristic of the turbulence. Turbulence is typically modeled with a two-equation non-linear  $k-\epsilon$  model that can capture secondary recirculation zones in corners. The turbulent fluid mechanics and chemical reactions are coupled using progress variables to track the turbulent mixing process. Gas-phase reactions are assumed to be limited by mixing rates for major species as opposed to chemical kinetic rates. Gaseous reactions are calculated assuming local instantaneous equilibrium.

The radiative intensity field is solved based on properties of the surfaces and participating media and the resulting local flux divergence appears as a source term in the gas phase energy equation. Our models include the heat transfer for absorbing-emitting, anisotropically scattering, turbulent, sooting media.

Particle mechanics are computed by following the mean path for a discretized group of particles, or particle cloud, in a Lagrangian reference frame. Particle reaction processes include coal devolatilization, char oxidation and gas-particle interchange. Particle reactions based on fuels other than coal can be modeled. The dispersion of the particle cloud is based on statistics gathered from the turbulent flow field. Heat, mass and momentum transfer effects are included for each particle cloud. The proper-

ties of the particle cloud are computed from a statistical average over the particles within the cloud. The properties of the local gas field are computed with an analogous ensemble averaging procedure. Particle mass and momentum sources are converted from a Lagrangian to an Eulerian reference frame by considering the residence time of each particle cloud within the computational cells. The resulting volumetric source terms provide the coupling of the dispersed phase particle mechanics and heterogeneous combustion to the gas phase fluid mechanics.

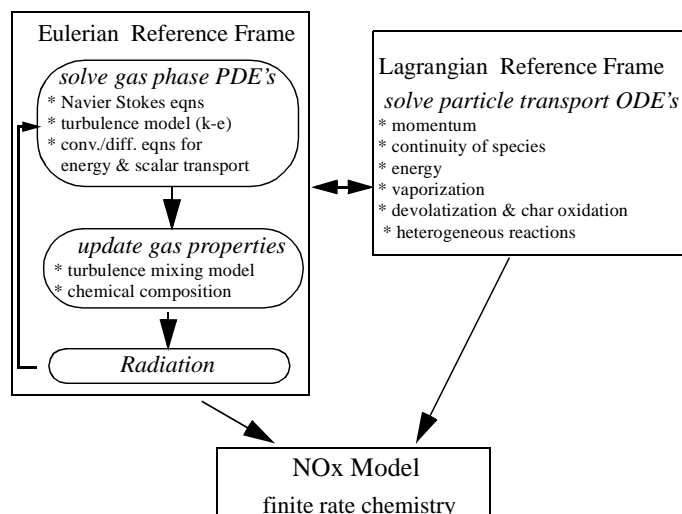


Figure 1. Two Phase Reacting Flow Model Solution Scheme.

The solution algorithm for two phase flow employs a series of macro-iterative loops over the particle and gas phases (see Fig.1). Within each gas phase macro-iteration loop, an iterative loop is performed over the governing PDE's for fluid mechanics, "chemistry" (i.e., fuel stream mixture fractions and their variances) and radiative transport in a sequential manner to obtain updated solution values. The number of macro-iterations over the particle phase is dependent on the strength of the two-phase coupling within the reactor to be modeled. The governing equations for the gas phase (momentum,  $k-\epsilon$ , and other scalar variables) are solved using a pressure-based, segregated variable scheme developed for low speed, variable density flows (SIMPLER). Gas properties are updated by first computing the local turbulent mixing, and then computing the chemical properties of the gas; for computational efficiency, chemical properties are interpolated from equilibrium tables that are parameterized by the local heat loss and fuel mixture fractions. The radiative intensity field is determined using a discrete ordinates method (S4 or S6 approximation). The particle phase is computed by solving an initial value problem for the mean trajectory and dispersion of a cloud of particles. Included in the system of ODE's are equations for: particle momentum; continuity of species; particle energy (including particle radiation, convection and chemical reaction); particle liquid vaporization; particle devolatilization; and char oxidation. The governing set of ODE's is solved using a time-accurate predictor-corrector method for stiff

ODE's. Overall, this solution method provides a flexible, efficient and robust model for computing turbulent reacting two phase flows.

The rates governing the formation and destruction of NO<sub>x</sub> are significantly slower than those governing the primary heat release reactions. Thus, the assumption that these species are in local chemical equilibrium leads to accurate predictions of their local concentrations. To account for the finite-rate of formation of these species, additional equations governing the formation of thermal, prompt and fuel NO<sub>x</sub> are solved. The locally computed mean velocity field, and the mean and variance of the temperature and composition fields are used to determine the rates of formation and destruction of NO<sub>x</sub>. In this manner, dependence on local temperatures, radical species concentrations and stoichiometry are accounted for. The NO<sub>x</sub> chemistry has a negligible effect on the local temperature and velocity fields, hence this analysis can be de-coupled from the solution of the turbulent flow field and performed as a "post-process" for computational efficiency.

The number of iterations required for convergence is generally problem dependent. The convergence criteria is computed from the residuals of the discretized equations being solved. However, rather than using the equation residual directly, the level of convergence is reported to the user based on an estimate of the number of significant digits of accuracy in the solution. For academic test problems, such as isothermal flow or a single burner in a box, the model can be converged to about five digits of accuracy. For industrial problems with multiple burners and complex geometries the convergence usually is not as high. For a gas-fired furnace (i.e., single phase flow), convergence to approximately four digits of accuracy is usually obtained. For reacting two phase flow problems, typically only between three to four digits of accuracy can be achieved in the final solution. The number of iterations required for convergence is greatly reduced for a parametric simulation that is started from a previously converged baseline firing condition. For a gas-fired system, a parametric simulation can be converged in about 500 iterations in the gas phase (ie, Eulerian Frame). For a two-phase flow problem, restarted from a converged baseline simulation, a converged solution is typically obtained in ten to twenty (macro) particle iterations in which fifty to one hundred gas phase iterations are performed between each particle iteration. With regards to grid convergence studies, although this is a very useful test procedure for simple problems, when modeling complex industrial problems there is rarely sufficient time, computer resources or project funding to perform such studies. Hopefully, in the future with the advent of faster and cheaper computers, this will no longer be the case.

The computational models described above have been ported and optimized for use on PC's. A parametric case study for models presented in this paper can typically be obtained in 24-48 hours of cpu time on a PC with a DEC-Alpha processor.

## ETHYLENE PROCESS FURNACE

Ethylene production is a cornerstone of the Chemical Process Industry. Cracking furnaces typically consist of a long, relatively narrow furnace (radiant firebox) containing a large number of coils (process tubes) and a large number of gas burners. The purpose of the cracking furnace is to heat the process fluid (raw chemical feed stock) to a high cracking temperature to selectively produce ethylene while minimizing coke formation. With respect to operation, this requires obtaining a target heat flux to each tube, which in turn generally results in a complex coil pattern within the furnace. From the operators perspective, a key parameter is the Coil Outlet Temperature (COT). Obtaining uniform COTs for a furnace can require a significant amount of "field tuning" of operational parameters and thus additional expense for the furnace manufacturer and loss of production for the plant.

Based on previous work [8], REI developed a computational model specifically for cracking furnaces that included a tight, two way coupling of the heat transfer between the radiant firebox (furnace) and the process tubes. To accurately predict heat transfer to the process side fluid, the fire-side conditions must be coupled with the process side. The energy absorbed into the process coils acts to heat up the fluid and provide energy for the endothermic cracking reactions. Within the computational model, the temperature and composition of the fluid within the process tube can be approximated either using a CHEMKIN calculation or, as is more commonly done, using a customer-provided correlation that relates the accumulated heat transferred to the process tube with the temperature of the process fluid. It should not be overlooked that the process temperature affects the convective heat transfer on the inside tube wall as well as the outside tube metal temperature and finally, the net heat flux to the coil. Thus, the process and fire-side conditions are tightly coupled and must be modeled as such..

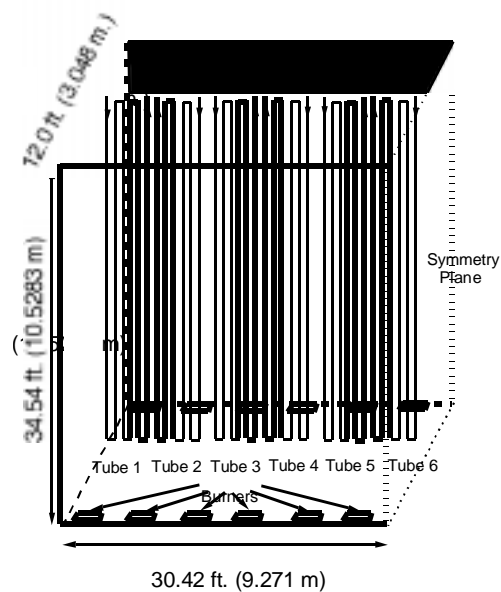


Figure 2. Schematic of Ethylene Furnace.

Illustrated in Fig. 2 (see previous page) is a section of an ethylene furnace that has been recently modeled [9]. The overall furnace dimensions are 60ft. x 30ft. x 10ft (LxHxD). Due to the symmetry of the radiant firebox, only one-half of the furnace was modeled. The computational grid consisted of 253x49x29 (LxHxD) or about 359K cells total. The furnace contains twelve simple serpentine M coils aligned vertically in a plane passing through the center of the furnace. Each coil consists of three vertical inlet passes or tubes and three vertical outlet passes. The firebox is floor-fired and the complete furnace contains 24 burners distributed in two rows placed adjacent to the furnace walls. The burners are spaced so that the centerline of each burner corresponded with the centerline of the opposing process coil. Thus, the burners have a non-uniform spacing within the firebox. The burners are nonpremixed staged gas burners with internal flue gas recirculation.

Illustrated in Fig. 3 is the predicted wall temperature within the radiant firebox and the predicted Tube Metal Temperature (TMT) for the process tubes or coils, for normal firing conditions. The predicted Coil Outlet Temperatures (COTS) for the same firing conditions are shown in Fig. 4. All simulations for this furnace indicated the presence of a significant cool end wall effect at a constant firing rate and constant flow to each coil. Fig. 4 shows that a variation in COTs of approximately  $\pm 10^\circ\text{F}$  can be expected with the third and fourth coils from the end wall yielding the highest COT and the first coil, the lowest. This variation is related to the distribution of refractory wall temperatures and the local gas temperature.

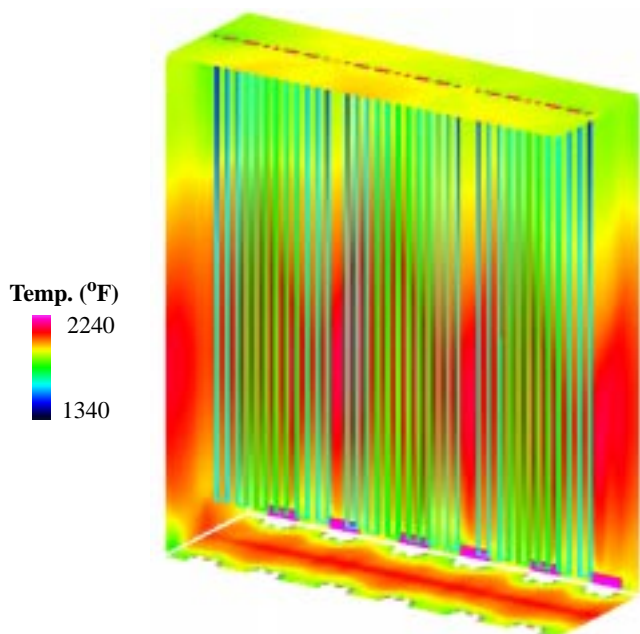


Figure 3. Wall and TMT for ethylene furnace

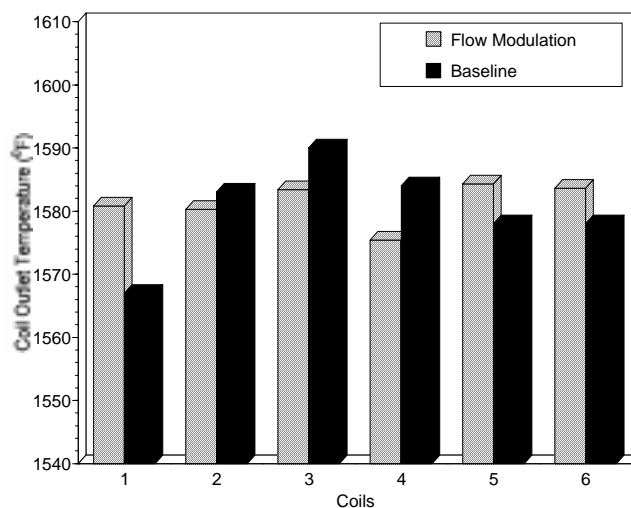


Figure 4. Comparison of predicted COTs with and without process flow rate modulation. In the baseline case, the coil flow rates are uniform. Pair-wise flow rate modulation denotes changes to flow rates to adjacent coil pairs.

Also shown in Fig.4 are the results for a simulation to try to achieve uniform COTs by independently adjusting, or modulating, the mass flow to each process tube [9]. The adjustments are performed with the stipulation that the total mass flow rate into the coils is not changed. The degree of modulation was based on the energy transferred to each pair of coils in the baseline simulation of normal firing conditions. The flow rate modulation to adjacent coil pairs did not exceed 1.3% of the baseline mass flow rates. From Fig.4 it can be seen that a nearly uniform COT distribution was achieved. Field tests have shown that this approach will work, but that the required modulation is approximately 5%. This discrepancy is in part due to differences in the provided versus true operating conditions. In the computer simulations it was assumed that the burners were fired uniformly and that the inlet process fluid temperature to the coils was uniform. However, in the field tests it was discovered that zonal firing of the burners is used in the furnace and that the process fluid temperature at the coil inlets varied by up to  $\pm 20\text{F}$  from the assumed value.

As described above, using a computational model can provide for a detailed examination of the effects of design and operating changes on process side conditions. In addition, nonlinear effects associated with changing firing rates, coil and furnace geometry, firing distribution, feedstock, and process flow rates can be examined in a rigorous manner. Computational studies can be performed while the furnace is still in the design stages. For existing furnaces, studies to improve performance can be conducted without impacting production.

## CYCLONE BARREL

Coal is the most commonly used fuel for power utility boilers. Conventional boilers burn pulverized coal within the furnace. One alternative to pulverized coal units are cyclone furnaces in which a coarser grind coal is pre-combusted in a barrel and only the resulting hot combustion gases enter the furnace. Cyclone furnaces avoid the high cost of using pulverized coal, allow the use of less expensive grades of coal and the use of alternative fuel sources. In addition, cyclone furnaces can have fewer fouling and slagging problems within the boiler because the fuel is pre-combusted. A significant drawback to cyclone furnaces is the high NO<sub>x</sub> content of the furnace flue gases. Low NO<sub>x</sub> firing systems typical of pulverized coal fired boilers may not be applicable to cyclone-fired boilers because of their unique design. Selective catalytic reduction, selective non-catalytic reduction and reburning technologies can reduce NO<sub>x</sub> emissions from cyclone-fired boilers, but at high capital and/or operating costs. With support from the Electric Power Research Institute (EPRI) sponsored NO<sub>x</sub> Control Interest Group (CNCIG), REI has developed a cyclone barrel computational model to evaluate standard barrel operating conditions and to investigate NO<sub>x</sub> reduction strategies [10].

The cyclone barrel model was developed by extending the two phase CFD model described above to include the features that are necessary to describe the physical and chemical phenomena controlling combustion in a cyclone barrel. These were primarily associated with improved particle transport and depo-

sition models that enabled particle flow in the burner and their subsequent deposition and reaction in the slag layer.

Illustrated in Figs. 5a-c are the gas temperature field for a ten foot diameter barrel that is fitted with a radial burner and fires a 70/30 blend of Powder River Basin/Illinois No. 6 coal [10]. The computational model consists of a 77x63x60 cell grid (291K cells). The flow field in the cyclone barrel is dominated by the secondary air flow which enters tangentially as do the coal and primary air streams in the radial burner. All three streams rotate in the same direction but the primary air stream is directed at the point at which the vertical coal chute enters the burner. There are two recirculation zones within the barrel, one at the exit of the burner and the other along the wall of the cyclone close to the burner end wall. The general flow is tangential until the gases accelerate axially as they exit the divergent throat. Since all the secondary air enters through a single duct, it is not surprising that the flow field is not symmetric. The gas temperature field shown in Fig. 5 illustrates the highly stratified flow that exist throughout the barrel. Even the gases exiting the divergent throat are not completely mixed. The secondary air flow rolls around the wall creating a scroll effect as it entrains the coal gases from the wall. The high temperature zones occur on the boundary of the air stream as it mixes and reacts with the rich coal gases.

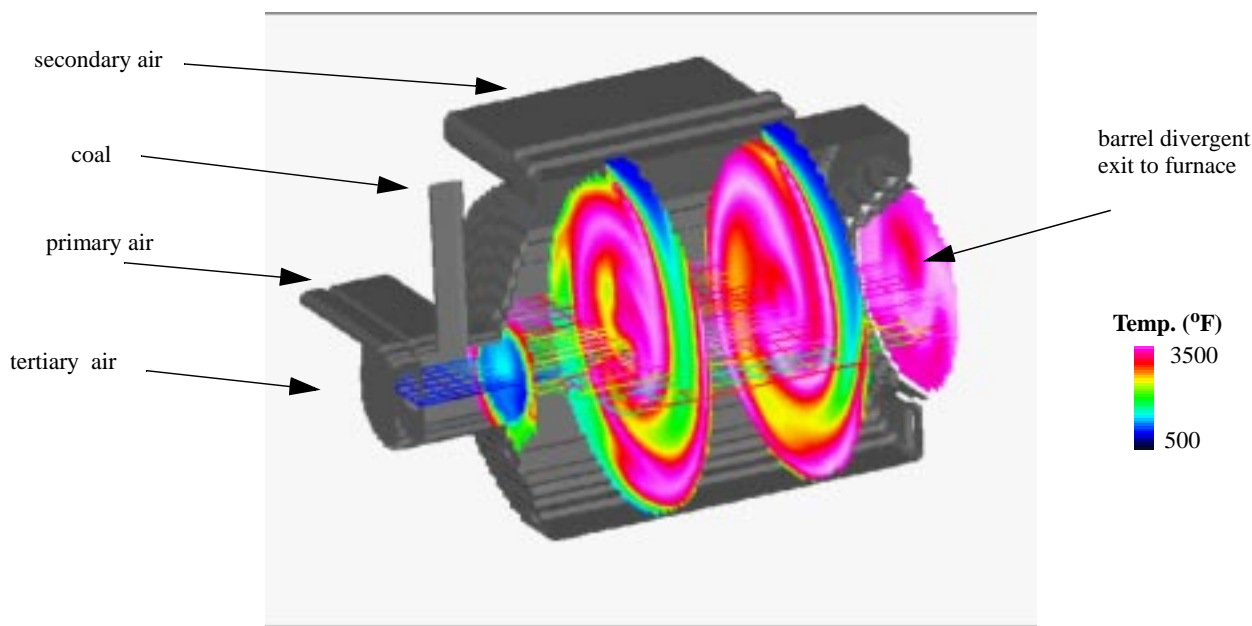


Figure 5. Gas temperature in coal fired cyclone barrel.

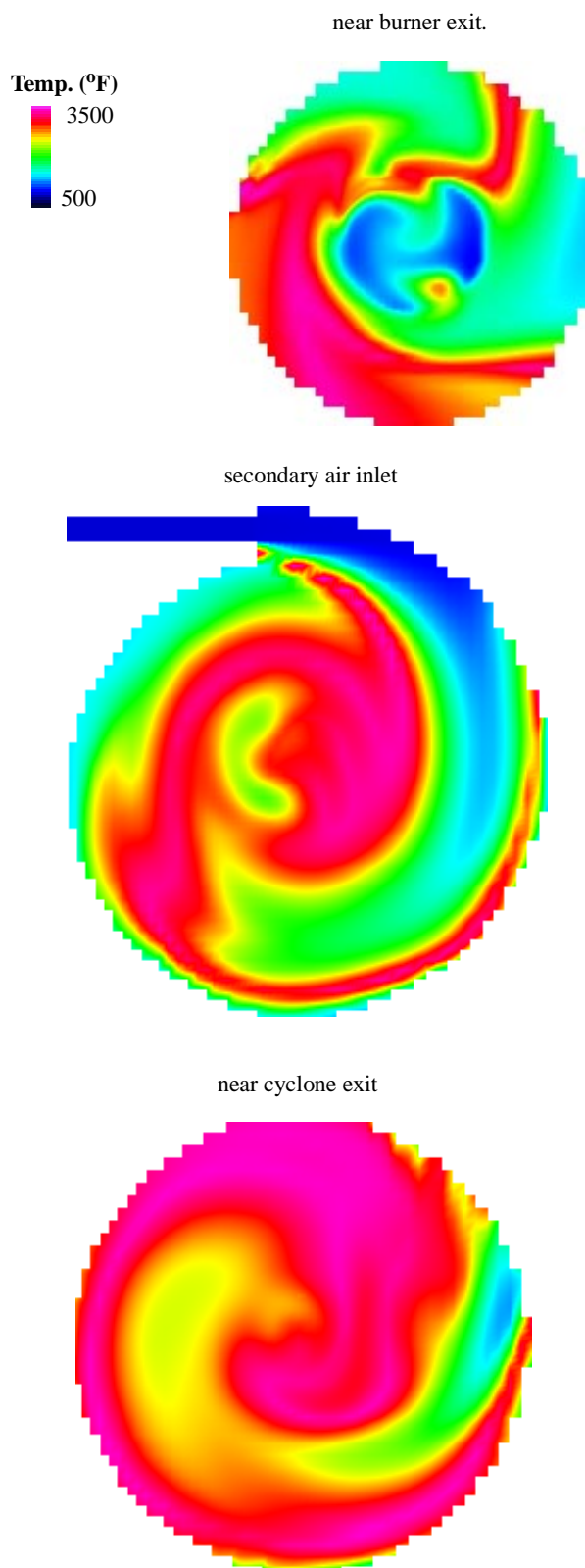


Figure 5b. Gas temperature in coal fired cyclone barrel.

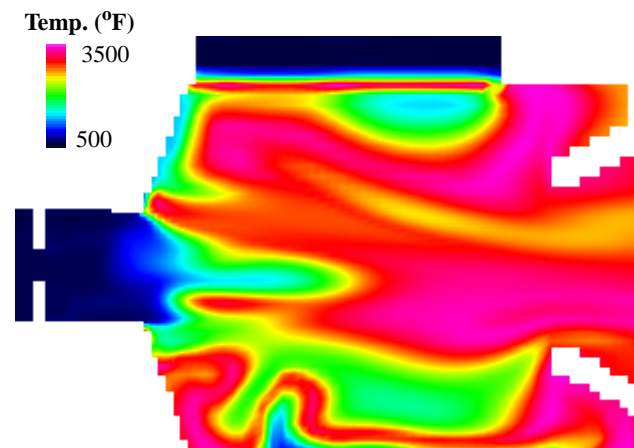


Figure 5c. Gas temperature in coal fired cyclone barrel along barrel centerplane.

Shown in Fig. 6a-c are comparisons of measured data with the computed gas temperature, oxygen, CO and NO concentration. The probe path angled down from the top of the burner to the bottom of the divergent exit and the data are shown as a function of probe insertion distance along this path. Data were obtained from several barrels operating at the same nominal conditions over a period of several days. Two data sets are shown for the measured oxygen concentration corresponding to measurements taken on different days but in the same barrel. Considering that the model indicates very steep gradients in both temperature and species concentration throughout the barrel, the agreement between the measured data and computed results is very good. The qualitative trends are in very good agreement and the quantitative agreement is acceptable. Little effort was expended to improve the agreement between the data and the predictions because it was felt that, considering the complexity of the cyclone combustion process and the difficulty of ensuring that the cyclones operate at fixed and known conditions the level of agreement was more than sufficient to validate the model. Additional comparisons for predicted and measured values for other cyclone barrels and for a cyclone barrel fired-furnaces are available in [10]

The computational model of the cyclone barrel has proven to be a valuable tool. As described above, comparison of model predictions with a data set of measured temperature and gas species concentrations indicated very good qualitative agreement and acceptable quantitative agreement. Model results show the cyclone to be poorly mixed and very stratified with large regions which are either very fuel or air rich. More important though is that by using the cyclone barrel model, NO<sub>x</sub> control options that involve simple variations in barrel operating conditions could be explored [10]. Some of these options have been tested and implemented in cyclone boilers by members of CNCIG.

### COPPER SMELTER FURNACE

A wide variety of process furnace designs are used in the mineral process industry. Illustrated in Figure 7 is a computational model of a copper cyclone reactor. In a copper smelting plant, cyclone reactors can be used to smelt the copper concentrate before its introduction into a settling furnace. The cyclone reactor is a major component in the smelting process and must operate at specific conditions to allow efficient and cost-effective plant operation. Common problems that inhibit optimal performance include buildup of accretions on the cyclone walls, mechanical dust carryover from the reactor into the settling furnace and surface damage to the reactor walls from heat or corrosion. Because the reactions occurring inside the cyclone reactor involve many coupled physical processes, it is difficult to know which process is causing the various operational problems and therefore which process to change. Hence, the development of a computational model.

The computational model of the cyclone shown in Fig. 7 was developed by extending the REI two phase reacting flow model to account for the reaction of copper sulfide concentrate within the cyclone reactor. Particle trajectories, temperature and reaction rates were predicted for a variety of furnace geometries and firing conditions. Appropriate sulfur chemistry was used to model sulfur evolution from copper concentrate and SO<sub>2</sub> formation. Simulations have indicated the principle mechanisms governing system behavior included sulfur kinetics, local particle temperatures, radiation, and appropriate coupling between these mechanisms.

Model predictions showed accretion buildup can be correlated with the rheology of particles deposited on the walls. Accretions are formed by deposited agglomerations of unreacted and partially-reacted particles. Initially a sticky material is formed on the cyclone surface, usually from molten flow on the walls, or from sticky particles deposited in these regions. Once the sticky base is provided, relatively cold (unreacted particles) may stick to the surface as well as hotter (more reacted) particles. If this agglomeration of particles does not reach temperatures sufficient to become molten (i.e., flow down the wall), a large accretion can form. If the region remains sufficiently hot, the material on the walls will become viscous and a slagging flow down the walls will occur. Tracking the time-temperature history of the particles that impact the walls provides a means of identifying regions of potential accretion buildup. Parametric studies of altering oxygen injection within the tuyere burners and the impact on accretion/particle deposition showed good agreement with field observations for comparable parametric variations in operating conditions within the reactor.

Detailed tracking of the particle clouds must also be performed to accurately predict mechanical dust carryover. By definition, carryover is the mass fraction of particles exiting the cyclone with the gas flow. By design, a large portion of the particles are captured onto the reactor walls. A sophisticated particle cloud transport model is required to accurately predict both the deposition and carryover of reacting copper. As is the case in traditional cyclones, it is the smallest particles (< 20 microns)

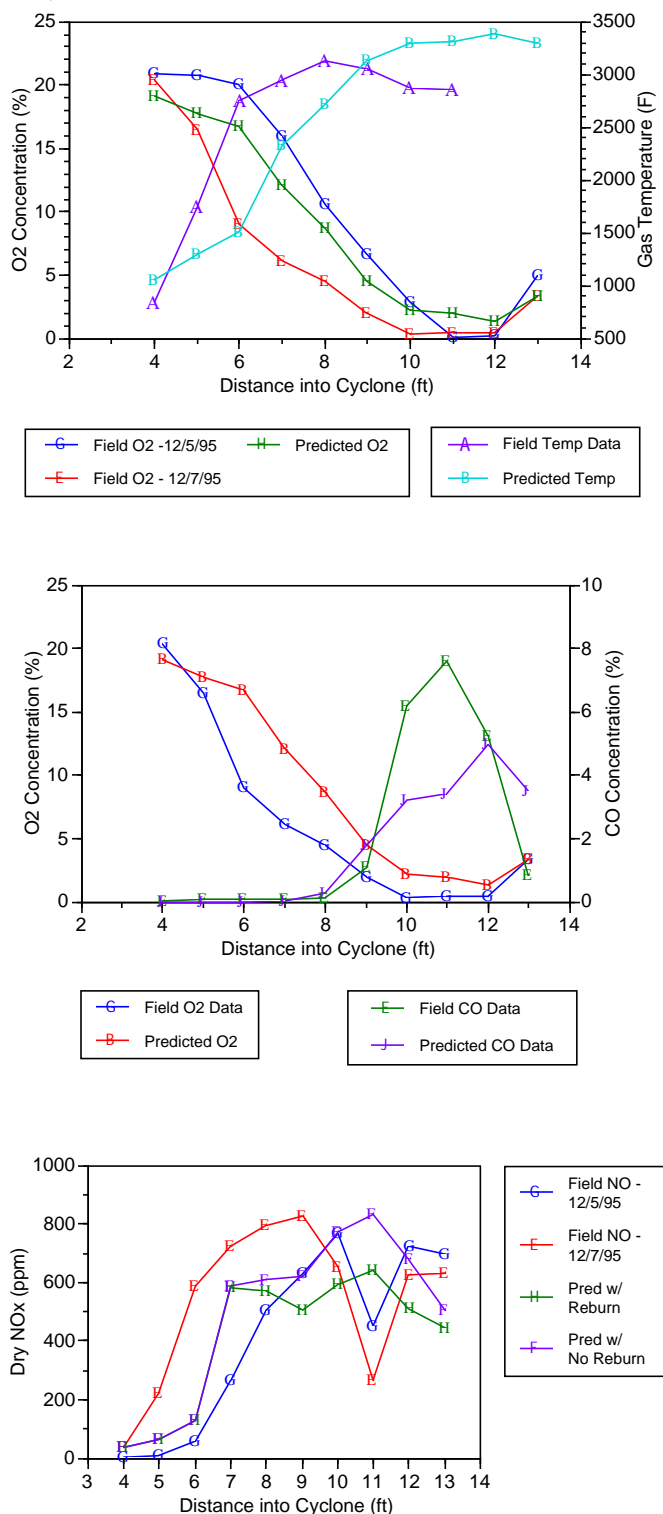


Figure 6. Comparison of predicted and measured gas temperature, O<sub>2</sub>, CO and NO concentrations in cyclone barrel.

that typically form the dust carryover. This is due to the relative difference between the centrifugal and fluid drag forces acting on the particles. The trajectory of the larger particles is driven by the centrifugal forces created by the cyclonic flow field, resulting in the large particles being thrown toward the reactor walls. In contrast, for the smallest particles, the dominant forces are due to drag and thus these particles tend to follow the rotating gas flow that exits the reactor. The dust carryover predicted by the computational model correlated well with estimated values determined by the plant engineers .

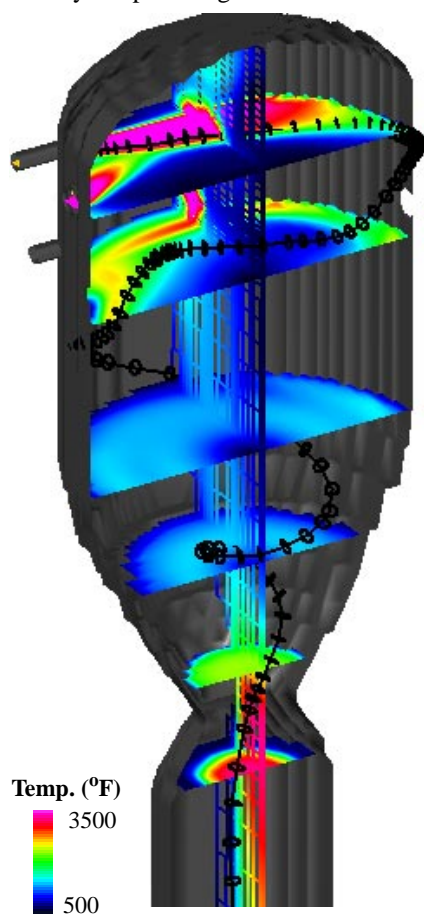


Figure 7. Cyclone reactor flow field. Shown is gas temperature at three horizontal planes. Also shown are the mean trajectories and dispersion of two particle clouds. The circles enclosing the particle trajectories indicate cloud dispersion.

Surfaces within the cyclone reactor are susceptible to damage by corrosion and warpage from heating effects. The corrosion on the walls is induced by locally reducing (oxygen lean) environments. In the computational model, the regions of potential corrosion problems can be readily identified by computing the stoichiometry of the gas field adjacent to the surface and easily identified/observed using standard 3D data visualization packages. Reactor wall warpage can occur due to localized hot spots. Many of these hot spots occur in regions opposite of the tuyere burners within the cyclone. These hot spot regions can be identified by plotting the predicted wall temperatures.

Working closely with plant personnel, the computational model of the cyclone was "validated" by comparing the trends observed in the model with field tests for similar variations in operating conditions within the operating cyclone. Although the plant data was only qualitative, the general trends were in very good agreement. Using the computational model, additional simulations were performed to test alternative operating conditions and reactor design changes. The simulation results have been used to redesign the cyclone to improve reliability and throughput.

## CONCLUSIONS

In this paper we have presented the results from computer simulations for three different industrial furnaces using a CFD-based two phase, reacting flow model. For all of the modeled systems, comparisons with qualitative data from plant personnel have been performed. Where available, comparisons with quantitative field data have been provided. Overall, the models have good agreement with qualitative trends and acceptable agreement with quantitative data.

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