# Remote Engineering Tools for the Design of Pollution Control Systems for Commercial Boilers

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## 1 Introduction

Applications from commercial engineering problems are often extremely complex and involve extensive collaboration between a diverse group of people to ensure their effective solution. An essential component of these collaborations is the ability of everyone involved, from computational scientists to field engineers, to be able to interpret, interact with, and optimize the computational model. Immersive virtual environments represent a promising new technology that facilitates these collaborations and as such are beginning to play an important role in the computational modeling of commercial engineering problems.

In this paper, we discuss a pilot project involving a collaboration between Nalco Fuel Tech (NFT), a small company that has developed state-of-the-art emission reduction systems for commercial boilers, and the computational science group at Argonne National Laboratory (ANL). The key objective of this project is the development of a real-time, interactive capability that allows the user to drive the computational model from within the virtual environment. In this case, the required interaction involves the placement of chemical injection systems in the boiler and a quick evaluation of their effectiveness in reducing undesirable emissions from the combustion process.

The numerical model of the combustion process and its interaction with the chemical reactions used to reduce emissions is complex, and the solution is computationally intensive. The timely solution of these models depends on advanced numerical methods and the effective use of high-performance computing resources. Our approach includes an implementation of an injector model that can be run on a variety of architectures ranging from the IBM SP to networks of workstations. This calculation is separate from the visualization process and numerical results are communicated to the virtual boiler using the CAVEcomm message-passing library developed at Argonne National Laboratory [4]. The virtual boiler environment consists of several components designed to aide in the efficient optimization of the injection system. In this paper we discuss the software that allows rapid virtual boiler construction, various mechanisms for data visualization, and a package for the interactive placement of injector nozzles.

Once the computational design process is complete, engineers are sent to the boiler site to install the injection system. Often during this phase, the onsite engineers encounter unforeseen obstacles that prevent placement of the injectors in the locations designated by the initial design. In this case it would be highly beneficial for the onsite engineers to quickly collaborate with the offsite applications expert to redesign the system. For this to be effective, the onsite engineer and the offsite applications expert need to simultaneously interact with each other and with the computational model as though they were in the same location. The technological challenges that need to be addressed include the incorporation of new information into the model, real time transmission of scientific data from the computational model to the virtual environments, and management of the collaborative interaction of the on-site engineer with the applications expert.

The Information Wide Area Year (I-WAY) [2] and Global Information Infrastruc-

ture (GII) testbed deployed at the Supercomputing 95 (SC95) conference provided an excellent opportunity to study the utility of such a remote engineering tool. In this paper we describe an experiment in which two scientists who are located 3000 miles apart collaborate together to design the pollution control system for a virtual tire incinerator. The CAVEcomm library allows the local system to be easily extended to include multiple CAVEs and remote access to the data from the computational model. The I-WAY network provided the bandwidth necessary to handle the real time transmission of scientific data from a remotely located supercomputer to the two CAVE environments.

We have organized the remainder of this paper as follows. In §2 we present the computational model used to simulate the physical processes withing the boiler. Particular attention is given to the modeling of particle trajectories and nozzle sprays. The approach we have used to visualize and interact with the computational model in the CAVE environment is discussed in §3. In §4 we discuss the use of the CAVEcomm library and I-WAY network as the communication layer between the numerical model and one or more CAVEs. Finally, in §5 we summarize the current state of this project and discuss future research directions.

### 2 Modeling the Emissions Reduction Process

The nitrogen oxide emissions reduction system modeled in this project works by injecting a chemical reagent into the combustion chamber of an operating boiler. The chemical reagent is effective only if it is injected within the bounds of a limited temperature window. If the temperature is too low, the reactions do not occur and the nitrogen oxides are not reduced; and if the temperature is too high, undesirable ammonia byproducts are formed. Thus a full understanding of the velocity fields and temperature distributions within the boiler is critical to the design of these systems.

A detailed and accurate computational model that allows engineers to study phys-

ical processes occurring within the boiler is a principle component in the design of the pollution control systems. The model is comprised of several distinct parts: (1) the specification of the boiler geometry and site-specific boundary conditions; (2) the combustion process itself, the resulting temperature distribution, and the flow velocities; (3) the spray from the injectors, their dispersion and evaporation; and (4) the chemical reactions and kinetic interactions between the spray reagents and the combustion process.

The specification of the boiler geometry is usually done from engineering drawings because most operating boilers were designed and built prior to the advent of CAD modeling systems. We have implemented a flexible geometric modeling interface that allows for the specification of different boiler geometries. This geometric description is the basis for both the virtual boiler model and the discrete computational domain used to model the combustion process.

The modeling of the combustion process in the boiler involves the solution of a large computational fluid dynamics (CFD) problem derived from the boiler geometry, operating parameters, and specified boundary conditions. Currently, the commercial CFD code Phoenics [1] is used to compute the steady-state combustion solutions. The fluid flow solutions and temperature distributions obtained from the solution of the CFD models are used as the input for modeling the chemical reactions involving the injector systems [6].

The results of the chemical kinetics model for each injector configuration gives the predicted effectiveness of the pollution control system. Finding the optimal configuration of the injection system is an iterative process in which the only parameters that can be adjusted are nozzle location and specific spray configuration. This iterative design phase consumes the largest portion of the solution time. Therefore, the primary effort in this project has been to develop the particle models representing these sprays and to implement the virtual environment necessary to interactively place the injectors to optimize their performance. In the remainder of this section we discuss the numerical modeling of the particle systems.

#### 2.1 Computing Particle Dynamics

The dynamics of a particle in a flow depends on a number of physical properties of the flow including the fluid velocity vector field, fluid temperature, and density. In addition, a particle's dynamics is determined by its size, density, temperature, position, and velocity. Given these parameters, the particle models used to predict these dynamics are the basis of the spray injector models and can be used to visualize the flow field itself. To illustrate the computations required for the particle dynamics, we introduce the models used in the simulation.

The simplest case, massless particle paths, are calculated by simply following the computed fluid (in this case the flue gas) velocity field. We refer to these solutions as streamlines, and these are the paths used in flow visualization. The differential equation for a massless particle in a flow is given by

$$\frac{d\vec{x}}{dt} = \vec{V}_p \quad \text{with} \tag{1}$$

$$\vec{V}_p = \vec{V}_g, \tag{2}$$

where  $\vec{x}$  and  $\vec{V}_p$  are the particle position and velocity vectors, respectively, and  $\vec{V}_g$  is the fluid velocity vector given by the CFD solution data at the point  $\vec{x}$ . The integration of this system generates the streamline issuing from any initial point in the flow field.

An essential property of real particles is their mass. The effect of the particle's momentum when it is injected into the combustion chamber can result in a very different trajectory from that of a massless particle. The massed particle model uses Equation (1) and includes dependencies in the formula for  $\vec{V_p}$  for the forces on the particle resulting from fluid resistance and gravity. The system of equations governing

particles with mass is given by Equation (1) and

$$\frac{d\vec{V_p}}{dt} = \frac{18\mu_g(\vec{V_g} - \vec{V_p})}{\rho_p D^2} + \frac{\rho_p - \rho_g}{\rho_p} \vec{g}.$$
 (3)

Here,  $\mu_g$  is the viscosity of the fluid,  $\rho$  is the density, D is the particle diameter, and  $\vec{g}$  is the gravitational acceleration vector. The first term on the righthand side of equation (3) is the fluid resistance imposed on the particle. A more general form of the fluid resistance includes a coefficient of drag,  $C_D$ , and a Reynolds number,  $N_{Re}$ . This term is absent from equation (3) because we assume that the particle has a low Reynolds number and, hence,  $C_D N_{Re} = 24$ . The second term on the righthand side of Equation (3) is the acceleration due to gravity. Note that by using the difference between the densities of the particle and fluid, buoyancy forces are included in this term as well.

The injector sprays are composed of a large number of droplets containing aqueous solutions of reagent. These droplets are injected into the flue gases and quickly evaporate, thus releasing the reagents and allowing them to react with the  $NO_x$ compounds to form nitrogen, carbon dioxide, and water. To include the effect of evaporation in the model, we again use Equations (1) and (3). To efficiently account for the processes of heat and mass transfer, we make some simplifying assumptions. We assume that the evaporation is heat transfer limited and that the droplet heating time is short compared to the droplet evaporation time. Thus, the temperature of the particle rises to near its boiling point and then begins to evaporate. This process described by the equation

$$\frac{dT_p}{dt} = \frac{N_{Nu}\pi kD(T_g - T_p))}{(m_p c_p^p)},$$
(4)

where  $N_{Nu}$  is the Nusselt number, k is the thermal conductivity of the fluid,  $T_p$  and  $T_g$ are respectively the temperature of the particle and the gas, and  $c_p^p$  is the specific heat of the particle. Second, once a particle reaches its boiling temperature, we assume that all further heat gains from the fluid cause mass loss from evaporation without further changes in temperature. The evaporation is described by the equation

$$\frac{dm_p}{dt} = \frac{\left(\operatorname{Nu}\pi k D(T_g - T_p)\right)}{H_v},\tag{5}$$

where  $H_v$  is the heat of vaporization of the particle.

#### 2.2 Modeling Injector Sprays

We model injector sprays by computing the trajectories of a large number of evaporating particles through the flow field using equations (4) and (5). The initial speed of every injected particle is assumed to be thirty meters per second. The orientation of the initial velocity vector is randomly distributed with respect to the orientation of the injector. In this case, sample distributions are chosen using a Gaussian distribution so that 95 percent of initial directions are contained in a thirty degree cone centered around the injector nozzle.

The diameter of each particle is randomly sampled from a lognormal distribution. These distributions are defined such that sampled particle diameters have a 95 percent chance of being less than one and a half times the distribution mean,  $\mu$ . Moreover, the distribution mean  $\mu$  is a function of the angle from the cone center;  $\mu$  decreases linearly from 500 microns for an angle value of zero to 100 microns at the edge of the cone. Distributions for angle values greater than 30 degrees have a consistent mean of 100 microns.

### 2.3 Numerical Implementation

Given any of the systems of ordinary differential equations described in Subsection 2.1, one can obtain a particle's trajectory in the flow field by the numerical integration of that system. An explicit forward Euler scheme is used to accomplish this task. A subtle aspect of the numerical integration of these trajectories is the data interrogation required from a discrete representation of the flow. The boiler is a complicated

geometric object, and many different discretization schemes can be used in the numerical model. These can range from structured brick finite volume discretizations to unstructured tetrahedral finite element meshes. Thus, as the integration routine tracks trajectories through this volume, it needs to efficiently access flow data at any point in the domain regardless of the discrete representation of the data. Therefore, the integration routine has been designed to be independent of the particular volume discretization used.

Another aspect to consider is the fact that the flow field data can be required at any point in the domain, not just the discrete points of data given by the CFD model. To address this issue, we have developed an interpolation algorithm that calculates a quantity at a general point in the domain by using a weighted sum (based on a finite element representation) of flow data from nearby discrete points. The interpolation procedure enables the interpolated velocity fields to vary continuously between volume cells. This property ensures that the streamline trajectories are a smooth, accurate representation of the discrete data produced by the CFD model.

An important, practical aspect of the implementation of the particle integration program has been the use of portable makefiles. This portability allows for the building of the particle code on a wide variety of computer architectures. For example, we have installed and run this code on the IBM SP system, SGIs, and Sun workstations. All calculations described in this paper are performed on the IBM SP located at Argonne National Laboratory.

### 3 The Interactive Virtual Environment

To visualize and interact with the results of the CFD and particle tracking models, we have developed a software package composed of three primary components. The first component is a graphics package used to quickly and efficiently construct virtual boilers. Once the boiler geometry is constructed, it serves as a frame of reference for the second component of the package, the data visualization software. This component is used to obtain an understanding of the flue gas velocity field and temperature distributions in the boiler. Once these are understood, the final software component is used to interactively configure the system of injectors and calculate a representative spray from each nozzle. The second and third components of this system require real-time streamline and particle trajectory calculations from the software described in the previous section. The communication layer between the visualization environment and the numerical simulation is provided by the CAVEcomm message-passing libraries developed at Argonne National Laboratory.

The visualization environment is based on the CAVE technology developed at the Electronics Visualization Laboratory (EVL) at the University of Illinois at Chicago [3]. Users are immersed in the virtual environment by stepping into a ten foot cube that has stereo images projected onto two walls and the floor. Several users may be simultaneously immersed in the same virtual environment and interact with the same computational model. One user is tracked by an electromagnetic tracking system, and the image orientation is calculated with respect to the head position of that user. Objects in the CAVE are manipulated by the user, who uses a wand, a three-dimensional analogue of the mouse on current computer workstations.

### 3.1 Boiler Geometry

Using the CAVE environment, we have developed an engineering tool that scientists at Nalco Fuel Tech can routinely use in the design of their emissions control systems. The optimal configuration of the injective system is unique, depending on boiler geometry and load specification, and must be redesigned for each new unit studied. Thus, it is critical that the software developed for studying the combustion data in commercial boilers be both flexible and easy to use.

The first step in achieving this goal is the development of a software environment

that allows the rapid construction of several types of virtual boilers. To do this, we have defined features commonly found in boiler construction, such as waterwalls, superheaters, and ash hoppers, as fundamental objects in the software. To fully define the graphical representation, several attributes may be associated with each fundamental object. For example, an exterior wall is fully defined by the *n* vertices in space defining its polygonal shape, a texture image, its position and orientation and by a Boolean boundary attribute. By using this approach, a new virtual boiler unit can easily be constructed in less than a day.

Figure 1 shows the exterior of a virtual tire incinerator. In the real boiler, particulate matter is introduced into the combustion chamber through the large chute shown in the figure. Large gray header pipes on the exterior are used as storage and separation units for the water and steam that are circulated through the interior waterwalls.



Figure 1: The exterior of a virtual boiler

It is critical that the user have access to every compartment of the boiler to study all aspects of the velocity flow field and temperature distribution. Navigation through the boiler compartments is achieved by using the wand to control two different modes of movement, a flight simulator mode and a jet pack mode. The display frame rate associated with navigation through the boiler is increased by using several optimization techniques including clipping planes, interior/exterior spatial definitions, customized graphics objects, and display lists. In addition, the frame rate can be further increased by toggling an option that removes all texture maps and unnecessary features, leaving only a polygonal wireframe representation of the boiler walls. This wireframe representation is also useful for obtaining a global understanding of the computed data because it allows the user to view all chambers in the boiler simultaneously (see Figure **??**).

#### 3.2 Data Visualization

We use the virtual boiler geometry as a frame of reference for the display of numerical data available from the Phoenics CFD model. We have provided several options for data visualization that can be used to obtain insight into the numerical combustion velocity and temperature results. The entire flow field can be displayed by using an array of vectors (represented by tetrahedral darts) in which the direction coincides with the direction of the flow, the length indicates magnitude or speed of the flow, and the color corresponds to the temperature or any other scalar quantity such as chemical species concentration. This representation of the data is shown in Figure 2. Unfortunately, this data representation is often confusing and does not always provide an intuitive feel for the velocity field.

To address this problem and facilitate the study of interesting areas of the computational domain, we have developed an interactive system that allows the user to initiate a streamline from any position within the virtual boiler. The starting point of



Figure 2: The flow field displayed as an array of static tetrahedral darts

the streamline is given by the location of the wand at the time of initiation. This spatial coordinate is communicated by using CAVEcomm to the remote particle tracking process. Once calculated, the entire path of the particle through the boiler is returned to the visualization process.

The data representation of the streamline consists of a sequence of connected line segments which can be displayed in either a continuous or animated fashion. The length of each segment is directly proportional to the magnitude of the velocity of the particle at that point in its trajectory. Animation of the particle along the streamline is obtained by stepping through the endpoint positions of the line segments. The tetrahedral darts traverse the streamlines and provide an illustration of the true relative velocity of the particles. Figure 3 shows several continuous streamlines initiated from the combustion chamber.

The animated streamlines can be used as the basis of a dramatic demonstration



Figure 3: The flow field illustrated through the use of streamlines

of the large-scale structure of the flow fields in the boiler. Rather than choosing a single starting point, we choose a planar, two-dimensional array of initial points from a boiler cross-section. The particle streamlines are computed from this initial array of points, and the resulting animations are displayed simultaneously. In Figure 4 we show flow vectors soon after they have left the initial plane. One example of the effectiveness of this approach is that it clearly identifies recirculation zones in the primary combustion chamber, a large-scale feature of tremendous interest to NFT engineers.

### 3.3 Injector Modeling

Once an understanding of the velocity flow field and temperature distribution within the boiler is obtained from the CFD model, engineers design the system of injectors to reduce harmful emissions from the boiler. The initial injector placement within





the boiler is obtained primarily by using the knowledge of temperature distribution and flow field data from the computational model and the prior experience of an engineer who has worked with similar boilers. The emissions reduction for this initial system is calculated, and the injector configuration is iteratively refined until the target emissions reduction is obtained.

Up to twenty-five injectors can be placed on exterior boiler walls. Once an initial configuration is selected, the position and orientation of each injector is communicated to the remote particle tracking process. Using the statistical model described in Section 2, the trajectories of one hundred evaporating particles are calculated for each injector and communicated back to the visualization process. Figure 5 shows the spray from a typical injector. Animation of the spray is obtained by stepping through the calculated trajectory positions in the same manner as with the streamlines. Note

that the size of the each particle corresponds to that particle's current mass, which decrease as the particle evaporates. Additionally, the user has the option to color the injector spray temperature or by source to examine the coverage provided by each injector.



Figure 5: Two injector placed on an exterior wall showing an evaporating particle flow.

Optimization of the injection system is accomplished within the virtual environment by using tools that allow the user to select, move, and delete injectors currently in the model. Selection and relocation of an existing injector is accomplished by pointing the wand toward the targeted injector. The intersection point of the wand and the boiler walls is calculated and if it falls within a three foot square around the injector, the nozzle is highlighted as selected. The relocation of that nozzle is accomplished by simply dragging it to the new location. Once repositioned, the user need only request injector sprays and new and/or repositioned injector positions are sent to the particle tracking code and the trajectories calculated.

### 4 The Communication Layer

The optimal performance of the interactive system described in this paper is obtained when the numerical calculations are separated from the visualization software. Hence it is critical that these components be able to communicate with each other in an effective, low-cost manner. In addition, this communication layer needs to be portable so that the numerical calculations can be performed on a variety of architectures ranging from Sun workstations to the IBM SP. The CAVEcomm library [4] developed at Argonne National Laboratory provides the performance aspects needed from the software perspective, and we use this standard as our message-passing interface. Since we are sending a large amount of scientific data from the numerical model to the visualization environment, we require high speed networking links. An advanced, national high speed network, the I-WAY, was deployed at the SC95 conference held in San Diego and provided an excellent opportunity for examining the use of our tool for remote engineering applications.

#### 4.1 The CAVEcomm Library

The CAVEcomm communication library uses a client-server model in which a broker is used to mediate the communication between the particle tracking code and one or more CAVE environments. Each active component of the system must register itself with the broker and subsequently subscribe to the data streams it would like to monitor. For example, Figure 6 shows the interactions required between the CAVEcomm broker, the particle tracking flow model process, and the main CAVE process to start a single cave system. The steps are time ordered from top to bottom as shown by the arrow on the rightmost side of the figure. The initial connection to the broker is made by the particle tracking process's registration request. A visualization process is then started, registers itself with the broker, and attempts to subscribe to data from the flow model. All computation in the main CAVE process is blocked until a successful subscription is made. The CAVEcomm broker notifies the flow model that a subscription request has been made, the visualization environment is added to the list of subscribers, and the main cave process is notified of a successful subscription. Following this initial phase, the two applications are able to interact directly without mediation from the broker; the visualization process requests general information directly from the flow model and the velocity field data from the converged combustion model.



Figure 6: The communication interactions between the CAVEcomm broker, the visualization process, and the flow model process during startup.

To revise the computational model during the installation phase, the on-site engineer and the off-site applications expert ideally should be able to collaborate and interact with the computational model as if they were in the same location. The incorporation of a second visualization environment to allow these remote collaborations is straightforward using the CAVEcomm libraries. The initial mediation between the broker, the second cave, and the flow modeling process is identical to that used for a single cave start-up. The additional communication required to connect the two caves together are shown in Figure 7. The second CAVE sends a message to the broker and subscribes to the head and wand tracking data from the first CAVE. The first CAVE similarly subscribes to the tracking data from the second CAVE. This tracking data is then used to plot a representation of the user in the remote CAVE for which the head and wand placement and orientation are correct.



Figure 7: The additional communication required to add a second CAVE to the interactive system.

By default, the flow model process is subscribed to data from all of the CAVEs and broadcasts information to all CAVEs that request it. We note that once the flow model data is received by the CAVE, it resides in the local system so that the visualization remains independently controlled by the local user. Hence a user in one CAVE may be viewing data from static vector field and user in a different CAVE may be viewing animated streamlines that have been initiated.

To simplify flow model interactions, only one user is authorized to request data from the numerical simulation at any given time. By default, the first CAVE that subscribes to the numerical simulation is given the authorization to request data. One feature that is necessary for effective remote collaborations to be is the ability to pass control of the design process to the remote user. This transfer allows the collaboration proceed in a seamless manner and input from both users can be used to place the injectors in optimal positions rather than requiring one user to remotely direct another in the proper placement of injectors. The remote user can obtain control of data requests at any time without the consent of the current controlling user. This request for control causes a message to be sent to the numerical simulation giving the requesting CAVE id, and data requests are now accepted from only that user.

#### 4.2 The I-WAY

The bandwidth and latency in the current networking infrastructure are inadequate to handle the large amount of information that is transmitted between the particle tracking code and the remote user(s). This year at SC95 an experimental high-performance network called the I-WAY [2] was built linking supercomputing resources around the country with Asynchronous Transfer Mode (ATM) speed. This environment represented an ideal testbed for examining the utility and performance of the remote collaborative tool described in this paper.

For this experiment we connected a CAVE environment located on the SC95 show floor in San Diego, CA to a remote CAVE environment located at the Advanced Research Projects Agency (ARPA) in Washington DC. All computations from the particle tracking model were performed using the IBM SP located at Argonne National Laboratory in Chicago, Illinios. The CAVEcomm broker process was also run on the IBM SP at Argonne.

The I-WAY network used OC-3c links which operate at 155 Mbps or 15.5 times faster than fast ethernet bandwidth of 10 Mbps. As an example of the speed of this system, consider the initiation of a single streamline as described in Section 3. Each streamlines consists 4000 discrete data points that have four floats associated with each; three giving the spatial coordinate and one giving the temperature at that point. Thus there are 512000 bits of data to be transferred for each streamline which can be accomplished in .00330 seconds over ATM if latency is not considered. Empirical results from experiments on the show floor showed that performing the calculations and transmitting the results from several thousand miles away using ATM resulted in speeds comparable to those obtained using ethernet connectivity to a machine located a few feet away.

### 5 Summary and Future Work

We have presented an interactive tool that provides an effective mechanism for scientists and engineers at Nalco Fuel Tech to design emissions control systems for commercial boilers and incinerators. Several engineers can now work together in a CAVE virtual environment and directly interact with the computational model. This direct interaction coupled with the animated visualization features discussed in §3, allows the engineers to quickly interpret the numerical data from the CFD model and efficiently optimize the injector locations. In addition, the high speed networking capabilities provided by the I-WAY allow the possibility of remote collaborations in which high volumes of computational data are sent over an ATM network.

Several improvements are being incorporated into the current software environment that will improve its usefulness and increase the accuracy of the computational model. To facilitate the initial construction of virtual boiler geometries, we are defining a set of templates for common boiler types. Thus, rather than starting from a set of disjoint features, an engineer would begin with a boiler template and modify it as required to meet blueprint specifications.

To increase the capabilities of injector interactions, we are designing new tools that allow for the control of operating parameters such as droplet size and spray configuration. In addition, the particle tracking model used to model the sprays from the injectors can be improved in several ways. For instance, we can increase the resolution and hence numerical accuracy around the nozzle by incorporating unstructured mesh techniques such as those developed in the SUMAA3d [5] project. We can also improve the statistical accuracy of the model by using parallel processing to increase the number of droplet trajectories sampled and by incorporating a more realistic droplet evaporation model.

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