

TRENDS IN PREDICTING AND CONTROLLING EMISSIONS FROM COAL FIRED BOILERS

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ABSTRACT

The past decade has seen a dramatic increase in the use of computational fluid dynamics (CFD) in the solution of problems related to the design and operation of pulverized coal-fired utility boilers. Traditionally, there has been a major gap between the knowledge of coal scientists, who have over the past century made enormous progress in the characterization of coal and the processes it undergoes during combustion, and the application of that knowledge to the solution of practical problems. A well known practitioner often taunted the coal research community by saying, with some justification, that "the researcher's only contribution to the practitioner is to explain to him why he did what he did after he did it!" The advances in CFD and in computer visualization have made it possible to apply fundamental knowledge to the solution of real world problems and to translate the results to forms that are understandable and useable by the practitioners. A series of case studies will be presented on the application of fundamentals and CFD to characterize NO_x emissions, unburned carbon in fly ash, fly ash size and composition distribution, fouling and corrosion potential, and air toxics emissions, to illustrate the progress that has been made in the ability to solve real world problems with CFD. One can look forward to the day when computer simulations will guide the development and implementation of the next generation of clean and efficient coal-fired utility boilers.

INTRODUCTION

The challenges of meeting competitive and environmental targets can be guided by the use of computer simulations. This paper provides illustrations of how computer models are currently being used by the industry to solve some of the problems of trace element emissions. Although computer models for predicting furnace performance have been under development for some time, it is only recently that they have reached a state of maturity where industry is relying upon computer simulation to solve their problems.

A question that is becoming of greater interest in the U.S. is that of fine particles as the result of the recent promulgation of standards to control the ambient concentration of particles with diameters under 2.5 microns. The question here is how will the low-NO_x conditions influence the emissions of fine particles. Of greatest interest is the formation of the smaller particles in the sizes that penetrate the air pollution control devices (APCD) with relatively high efficiency, i.e., 0.1-1.0µm [Senior, et al., 1999a]. The transformation of mineral matter is dependent upon many factors including the size distribution of the coal, the combustion conditions, the forms of occurrence of the elements in the coal and the interaction of different elements.

The dominant constituents of coal mineral matter are iron, silicon, aluminum, the alkali and the alkaline earth elements. A schematic of how the minerals are distributed in coal, partially as included mineral matter, partially as atomically dispersed elements, and partially as extraneous mineral particles is shown in Figure 1. During combustion most of the mineral matter distributed in a coal particle is exposed on the surface as the surface of the char particles recede during oxidation. At the char surface, this mineral matter coalesces and forms one or more particles, usually in the 1 to 20 µm range, particles that will be captured with high efficiency by the APCD. However, a small amount, of the order of one percent of the ash in coal, will vaporize and subsequently recondense to form particles that are in the size range in which the penetration through the APCD is high.

The processes shown schematically in Figure 1 can be modeled. Figure 1 shows that part of the ash is vaporized and recondenses to form a submicron ash. Part of this vaporization occurs during devolatilization during which elements that are present in organometallic form, many of which are trace transition elements, are released. The refractory oxides (FeO, SiO₂, MgO, CaO) are vaporized by the reduction of the oxides to the more volatile suboxides or metals, the diffusion of the suboxides or metals to the particle boundary layer where they are reoxidized and condense to form a submicron aerosol [Quann and Sarofim, 1982]. The vapor pressure of the vaporizing suboxide or metal is determined at the higher temperatures by the equilibrium of the reaction between the refractory oxide (RO) and carbon monoxide (CO) inside the particle, or



The mass transfer from the surfaces of the mineral inclusions to the surface of the char particle determines the vaporization rate. The size of the submicron particles may be calculated from the mass vaporized using well-established theory on aerosol dynamics. In addition, as depicted schematically in Figure 1, the more volatile salts of the alkali metals and the volatile trace metals will vaporize. These will condense downstream of the combustion zone at points where the combustion products have cooled down to their condensation temperatures. They will deposit on the surfaces of existing particles, in a manner calculable from mass-transfer-limited condensation.

As mentioned previously, computational fluid dynamics (CFD) tools have been developed to the point where many practical problems of industrial interest can be solved. For coal-fired utility boilers, the problems are typically related to evaluating the viability of a modern retrofit, such as a low NO_x firing system, and evaluating the potential for adverse side effects such as increased levels of unburned carbon, additional deposition/fouling problems, and the potential for increased waterwall wastage. A case study will be presented here demonstrating how such CFD tools can be used to address a problem related to mineral matter transformations under low NO_x conditions. Because of the dependence of the vaporization of mineral constituents on temperature and local equivalence ratio, it is expected that staging for NO_x control will change the formation and emissions of fine particles. The temperature-oxidation history for individual particles provides the information needed for the calculations. Due to space limitations this paper will focus on presenting the transformation of mineral matter in ash to a sub-micron fume that transports air toxics.

METHOD

The development of a model for the vaporization ash was a two-phase process. Phase 1, the initial development of the model, is used to verify experimental data for single particle combustion. The second phase requires minor modifications such that multiple particles can be evaluated. Particle iterations such as this are common in advanced CFD codes used for modeling coal-fired boilers.

The development of the first phase of the model was necessary to verify this computational model with experimentally derived results. In this scenario, a particle temperature history was necessary for running the model. Since this data was not available from the experimental data, the information needed to be generated. This was done using coal properties and combustion conditions. This information was fed into a computer code, which calculates carbon burnout kinetics. These calculations provide the necessary information including particle size, temperature, and residence time. From this information, the vaporization of elemental ash inclusions can be determined.

The experimental results for ash vaporization were performed by Quann and have been documented in the literature (Quann and Sarofim, 1982). The model was run for 14 different coals used in the experimental analysis. Figures 2 and 3 summarize the results for the model cases as normalized against the vaporization determined by Quann. The code was used in calculating the vaporization for SiO_2 , Al_2O_3 , FeO , CaO , and MgO . However, due to space limitations the results are given only for SiO_2 and CaO .

As can be seen from Figures 2 and 3, the fourteen coals used in the model verification are referred to by their respective Penn State Coal Database number followed by the type, bituminous (B), subbituminous (SB), or lignite (L). It should also be noted that the vaporization when compared with Quann will vary depending on coal type and mineral inclusion size. Since the mineral inclusion size was not known for Quann's data, several cases were run. Agreement with Quann's data is observed for silica for the inclusion sizes of 10 to 20 μm , and for calcium for inclusion sizes of greater than 20 μm for the bituminous coals and less than 5 μm for the lignites. As will be discussed in the next section, coal 503-B will be used in actual multi-particle calculations. The values for the optimal inclusion sizes for each component for this coal are summarized in Table 1. The optimal inclusion size can be defined as those that are exactly verified with the Quann data.

RESULTS

The second phase of the vaporization had to be modified slightly to account for multiple particle iterations as performed in the CFD code. In addition, the code was run with and without the effects of CO_2 . In the comparison with the experimental results, the CO_2 was not an issue, but in an actual furnace case as will be shown, the CO_2 has a noticeable contribution.

The computational tools used in this study were developed by Reaction Engineering International (REI) to address a wide range of problems involved in the operation and design and of many combustion systems including utility boilers, pyrolysis furnaces, gas turbine combustors, rotary kilns, waste incinerators and smelting cyclones. The current models simulate both reacting and non-reacting flow of gases and particles, including gaseous diffusion flames, pulverized-coal flames, liquid sprays, coal slurries, injected sorbents, and other oxidation/reduction systems. Emphasis has been placed on simulating coal combustion and pollutant formation. This three dimensional, two phase reacting flow code (GLACIER) includes several capabilities necessary for accurate simulation of coal-fired boilers. These capabilities include turbulent particle transport with full coupling of particle and gas-phase mass and

momentum; coal reaction processes such as devolatilization, char oxidation and gas-particle interchange; NO_x formation/reduction chemistry; particle convection and radiation with absorption, emission and anisotropic scattering; full coupling of gas-particle energy exchange; and ash deposition. In addition, boiler-side waterwall and radiant panel surface temperatures can be predicted as part of the computation, given a backside (i.e., steam) temperature and surface resistance (from the deposit thickness and thermal conductivity, for example). As it applies to this paper, the vaporization model is actually a post-processor to be used in conjunction with the GLACIER software results.

The unit studied is a 500 MW opposed wall-fired boiler with twenty-four burners. Five wingwalls come in from the front wall. Prior to low-NO_x retrofit, the unit included Foster Wheeler's Intervane burners. During the retrofit, these burners were replaced by Foster Wheeler's Controlled-Flow/Split-Flame (CF/SF) burner. In addition, an advanced overfire air (AOFA) system was installed. This consists of an independent windbox for improved penetration/control of injection through eight directly opposed ports above each column of burners, and four underfire air ports at the level of the bottom burner row near the sidewalls.

As mentioned previously, the CO₂ was not an issue with the single particle model. However, under normal operating conditions, the CO₂ in the furnace plays a significant role. Figures 4 and 5 illustrate the cumulative vaporization for pre- and post-retrofit conditions accounting for effects due to CO₂ and neglecting the role of CO₂ respectively.

Since CO₂ is an issue which cannot be neglected it has been included in the current model for accurate calculation of the ash vaporization. Figures 6 and 7 illustrate the individual burner contribution to the total amount of ash vaporized. The symmetry plane has been identified, which is used in modeling the furnace in GLACIER. Also, the front and rear walls have been identified for both the pre- (Figure 6) and post-retrofit (Figure 7) cases.

DISCUSSION AND CONCLUSIONS

From these results it is evident that the modeling of ash vaporization is feasible. Additionally, it is apparent that the inclusion of CO₂ in the model is a necessary component. The presence of CO₂ ultimately suppresses the vaporization of ash as shown in Figures 4 and 5. Another aspect that is interesting to note is the variation in the vaporization between the front and rear wall. In the pre-retrofit case (Figure 6), the ash vaporization contribution from the front wall is 72 percent while the rear wall contributes only 28 percent. In the post-retrofit case, the contribution is more evenly distributed with 57 percent of the ash vaporized coming from the front wall and 43 percent from the rear. The next step in developing this vaporization model is to determine the particle size distribution of the vaporized ash.

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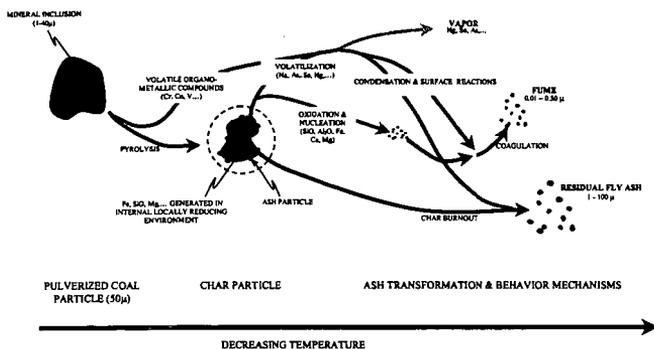


Figure 1: Schematic of Mineral Matter Transformation During Pulverized Coal Combustion.

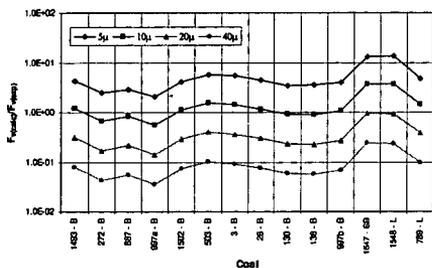


Figure 2: SiO₂ experimental results versus vaporization model.

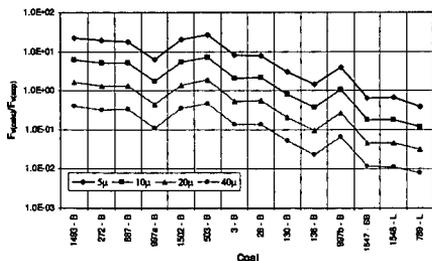


Figure 3: CaO experimental results versus vaporization model.

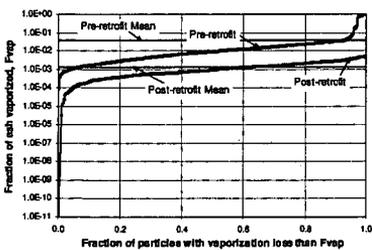


Figure 4: Cumulative vaporization for pre- and post-retrofit cases with CO₂ effect.

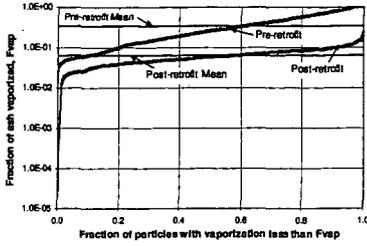


Figure 5: Cumulative vaporization for pre- and post-retrofit cases without CO₂ effect.

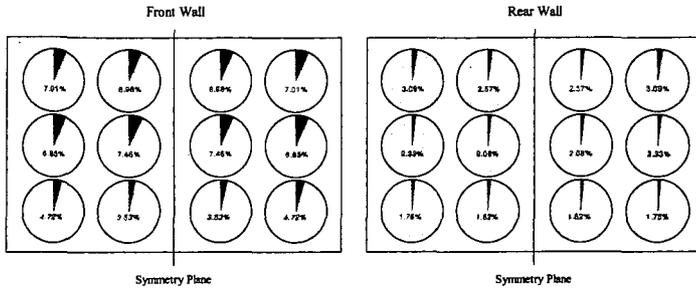


Figure 6: Pre-retrofit burner contribution to ash vaporization with CO₂ effects.

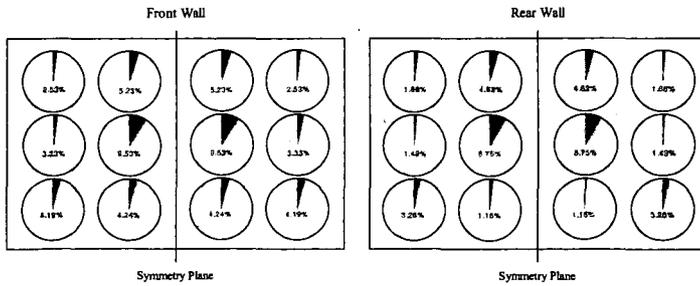


Figure 7: Post-retrofit burner contribution to ash vaporization with CO₂ effects.

Table 1: Optimal inclusion sizes for each ash component for coal 503-B.

Component	Optimal Inclusion Size (microns)
SiO ₂	13
Al ₂ O ₃	2
FeO	30
CaO	27
MgO	31