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**OPTIMIZED FUEL INJECTOR DESIGN FOR
MAXIMUM IN-FURNACE NO_x REDUCTION AND
MINIMUM UNBURNED CARBON**

by

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Introduction

In-furnace NO_x control techniques such as low NO_x burners, reburning, or hybrid approaches (e.g., reburning combined with SNCR) have proven to be the most cost-effective primary NO_x control strategy. This investigation focuses on two related applications of this technology, low NO_x burners and coal reburning. While these two approaches to NO_x control have been the subjects of numerous studies, two phenomena that could be important to future improvements are currently poorly understood – heterogeneous chemistry and two-phase mixing.

There are many low NO_x firing systems that have resulted in commercial units with significantly lower NO_x emissions [Sorge, 1992; Hardman, 1992; Sorge et al., 1993; Wingard et al., 1993; Marion et al., 1993; Pentersen and Lisauskas, 1993]. In summary, over twenty years of development have resulted in the demonstration of low NO_x firing systems for both wall and corner fired boilers. The following general conclusions of interest to this program can be made from past efforts:

- Unburned carbon levels tend to increase as NO_x emissions decrease.
- Development tests have consistently reported lower NO_x levels than field tests, due possibly to multiple burner effects, accuracy of control of operational variables, or differences in heat extraction rates.
- Increased heat extraction rates, which result in lower temperatures, tend to reduce NO_x emissions.
- Low NO_x burner designs emphasize fuel injector design to produce rapid ignition and to create optimal conditions for in-flame NO_x reduction.

Since the rate of decay of gas-phase total fixed nitrogen increases with temperature, it might be expected that NO_x emissions would decrease with increasing temperature in a fuel-nitrogen dominated environment. However, since the opposite is typically observed in practice, this effect was often ascribed to thermal NO_x . An alternative explanation has been offered by Takahashi and coworkers [1982] – the NO formed initially in the flame could undergo reduction by “active matter in the char.” A similar phenomenon has recently been observed in reburning studies. Chen and Ma [1995] attempted to separate homogeneous and heterogeneous effects during coal reburning and estimated that heterogeneous effects could be even larger than homogeneous effects in certain cases. This work is supported by the surprising effectiveness of wood as a reburning fuel despite the deficiency of CH_i radicals that are available [Brouwer et al., 1995]. NO reduction on char was always thought to be slow, but rates were measured on “old” char and, with the exception of DeSoete [1990], concentrated on direct reduction. Little information is available on char reactions under rich conditions in the presence of NH_i and HCN .

In addition to the role that heterogeneous effects play in NO_x reduction, they are important in understanding the behavior of unburned carbon levels during low NO_x firing. Char oxidation is the slowest step in the coal combustion process and therefore has been investigated in detail for a number of commercially important coals. However, until recently, chars have been assumed to burn at a constant rate regardless of temperature history or degree of conversion. Although this approach has proven adequate for describing heat release, description of burnout, where less than 1% of the fuel remains, may require a more sophisticated approach. Controlled laboratory studies [Hurt, 1993; Hurt and Davis, 1994] and examination of boiler flyash samples [Hurt et al., 1994] show that reactivities during the later stages of oxidation can decrease significantly due to crystalline ordering [Davis et al., 1994] or to preferential combustion of more reactive components [Hurt et al., 1996]. These results emphasize the importance of temperature/gas-composition history and suggest that a low- NO_x flame may be tailored to achieve optimal levels of unburned carbon.

Because of the importance of surface reactions to staged low NO_x burners and reburning, it is also necessary to improve the current understanding of the two-phase mixing processes occurring. Current low- NO_x firing technologies rely upon staging the fuel/air mixing at several levels (e.g., concentration of the fuel particles using coal spreaders in the primary stream or separation of primary and various secondary streams).

Most practitioners of reburning stress, that in practical applications, mixing of the reburning fuel with the products of the main heat release zone is an important consideration in the reduction of NO. Accurate descriptions of particle dispersion/concentration is important to improving the use of these techniques. The simplest of burner configurations result in a wide variety of flow patterns under varying conditions [Sheen et al., 1996] and much less is known about the relevant two-phase flow patterns.

The approach of this program is to proceed along five paths:

- Characterization of two-phase mixing environments simulating commercial low-NO_x burner designs in a water channel facility. This facility is equipped with an advanced Laser Induced Photochemical Anemometry system capable of accurately characterizing fluid and particle velocity fields simultaneously with particle concentration.
- Experimental evaluation of the reduction of NO by young chars under conditions typical of those encountered in low NO_x burners and reburning systems.
- Investigation of the structure of low-NO_x flames by characterizing particle and gas phase concentrations in the near field of relevant injector designs.
- Development of an advanced model of char burnout accounting for the effects of thermal annealing and coal heterogeneity.
- Use of a 3D, multiple phase, reacting CFD code to evaluate commercial burner designs and, after integration of the advanced carbon burnout model, to simulate boilers with existing field data.

Experimental systems for the two-phase mixing and char reduction experiments have been constructed and experiments are currently in their early stages. The work to be discussed herein will therefore focus on the following modeling tasks – the development of the advanced carbon burnout model and simulation of a commercial low NO_x burner.

Results

Advanced Carbon Burnout Model

An advanced Carbon Burnout Kinetic Model (CBK) has been developed with the following four main components or submodels:

- The single-film char oxidation model of Mitchell and coworkers [Mitchell et al., 1992; Hurt and Mitchell, 1992]. In the current version of CBK, the original published correlations have been modified to accommodate thermal annealing and statistical kinetic submodel integration and have been extended to include finite kinetics for lignites.
- A submodel of statistical variations in reactivity and char density among single pulverized fuel particles [Hurt et al., 1996].
- A submodel of thermal char deactivation, or thermal annealing, adapted from the model proposed by Suuberg [1991]. In this submodel the char reactivity is a variable whose value depends on temperature and time. CBK incorporates the thermal annealing model in full, differential form capable of accommodating a wide range of non-isothermal temperature histories. As discussed in detail elsewhere [Davis et al., 1995], the thermal annealing submodel is defined by three parameters: $\ln A_d$, mean $\ln E_d$, and $\text{sln} E_d$. These three parameters have been determined by comparison to a collection of thermal deactivation data from the literature, including recent data generated in collaboration with Imperial

- College [Beeley, et al., 1996]. Figure 1 illustrates the comparison using an optimized parameter set. A physical property submodel describing diameter/density changes during combustion, fragmentation, and mineral inhibition in the late stages of combustion.

The comprehensive CBK model was used in a series of one-dimensional reacting flow simulations to better understand the roles of the various individual phenomena described in the code on the overall prediction of carbon burnout. The thermal annealing submodel was found to have a large effect on reactivities and burnout levels at combustion temperatures and times typical of pulverized-coal fired boilers. The submodel of statistical kinetics and densities has a small effect throughout most of burnout, but contributes significantly to the long tails observed in laboratory burnout curves. Finally, the submodel of carbon/mineral interactions contributes substantially to the long burnout tails. None of these individual component submodels can be deleted from CBK without some loss of general predictive capability. For boiler applications however, coarse binning can be used in the submodel of statistical kinetics and densities without introducing significant error. The CBK model was successfully fit to six sets of long-residence-time data taken in the heated-wall reactor at Sandia. Typical results for two of these cases (the highest and lowest volatility coals) are shown in Figure 2. The global model predictions are shown again for comparison. Based on the results in Figure 1 and Figure 2, along with the original kinetic data presented in Mitchell et al, [1992], the single-particle temperature predictions in the statistical kinetic model [Hurt et al., 1996b] and the successful prediction of low reactivities in residual carbon samples [Hurt et al., 1996], it can be claimed that CBK describes all of the significant features of the Sandia char combustion database.

In order to prepare this model for integration into a comprehensive CFD code, careful sensitivity analyses were carried out in an effort to reduce the computational demands of the thermal annealing submodel. Numerous test cases were examined to find the optimal limits of integration and step size, considering both accuracy and speed. The total number of steps was reduced from 300 to 30, while maintaining an accuracy in deactivation factors within 3%.

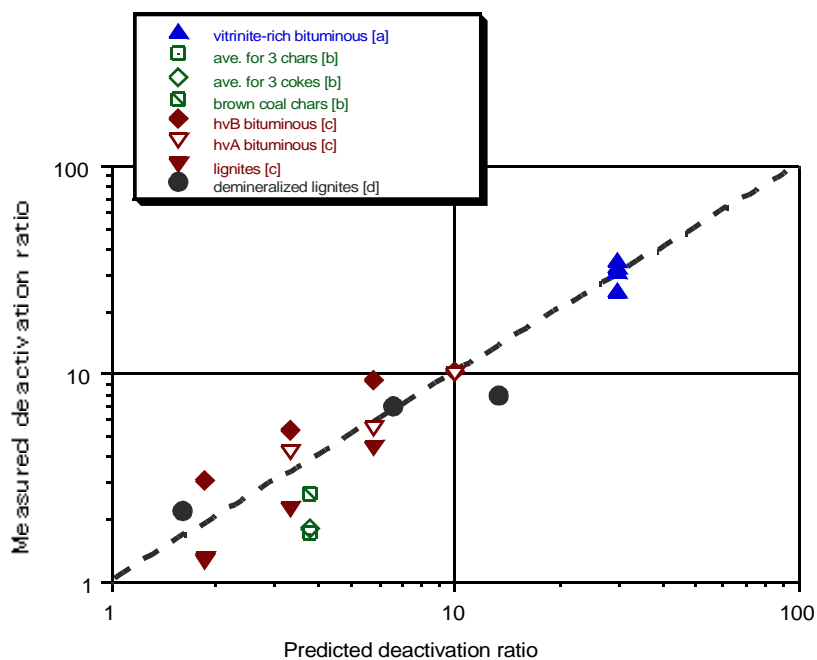


Figure 1. Comparison of predicted deactivation factors with measured values from the literature for a variety of char types and heat treatment conditions. Data sources: (a): Beeley et al. [1996]; (b): McCarthy [1982]; (c) Jenkins et al. [1973]; (d) Radovich et al. [1983].

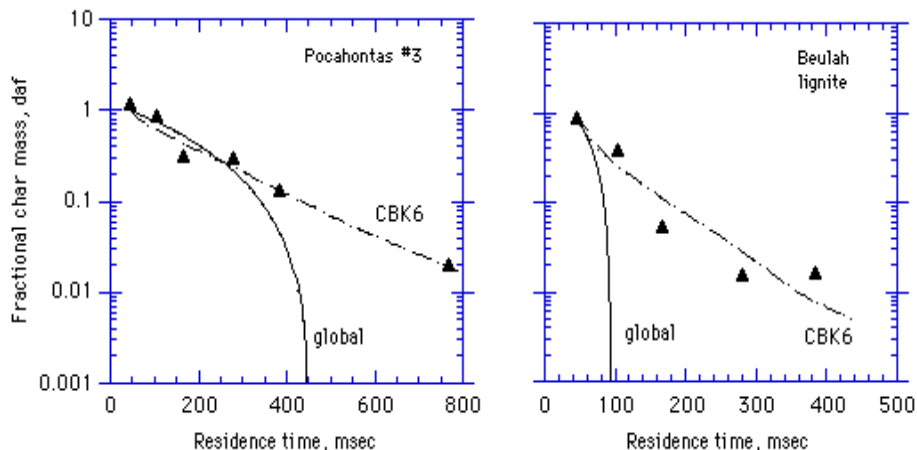


Figure 2. Comparison of measured conversion profiles from one-dimensional laboratory reactors (points) with predictions of the simple, global model of Hurt and Mitchell, [1992] (solid curves) and the CBK model (dashed curves).

Low NO_x Burner Modeling

Highly resolved modeling of the interior of a developmental low-NO_x burner has been performed. The burner under consideration includes a dual register burner and a coal pipe contain a venturi section and a four-bladed coal spreader. The modeling was performed in a non-reacting, isothermal mode for each of the three annular burner sections (primary, secondary and tertiary streams). In addition to the current state of the design, variations on the coal spreader blade angle and presence of the venturi were investigated. These design features have, under certain circumstances, proven to have a positive effect on NO_x emissions. Anecdotal evidence suggests that these two features serve to concentrate the coal particles and therefore lead to rich regions in which NO_x reduction is possible. Since these flow diversions will affect particles of different sizes to different extents, simulations were independently performed for particles that are extremely small (10 μ m), typical (60 μ m), and extremely large (230 μ m).

Figure 3 illustrates the magnitude of these differences for the current design. These images display particle mass density at the burner exit plane (each contour line represents a 10% increase). The difference in particle dispersion as a function of particle size is obvious, particularly for the 10 μ m particles. However, even these small particles show notable concentration into four lobes between the blades. The overall effect of the coal spreader and venturi appears to be to concentrate the particles into four lobes with the larger particles most prevalent at the center of the lobes. Quantitatively, 90% of the 230 μ m particles are concentrated in less than 1/3 of the cross-sectional area.

In order to isolate the effects of the venturi and of the blade angle, the same simulations were performed for (1) the same geometry without the venturi and (2) the same geometry with the blade angle doubled as illustrated in Figure 3 for the case of 60 μ m particles. The effect of the venturi is quite noticeable. Not only does the presence of the venturi concentrate the particles in the radial direction as one might guess, but it also appears to have a synergistic effect in terms of the effectiveness of the coal spreader and its concentrating effect in the tangential direction. The increase in blade angle also serves to further concentrate the particles. However, in this case the effect occurs in the tangential direction such that the nature of the tangential distribution is noticeably altered. (The contours go from peanut-shaped to pear-shaped.) The effects of the venturi/blade angle changes on the distribution of 230 μ m particles is similar to that of the 60 μ m particles.

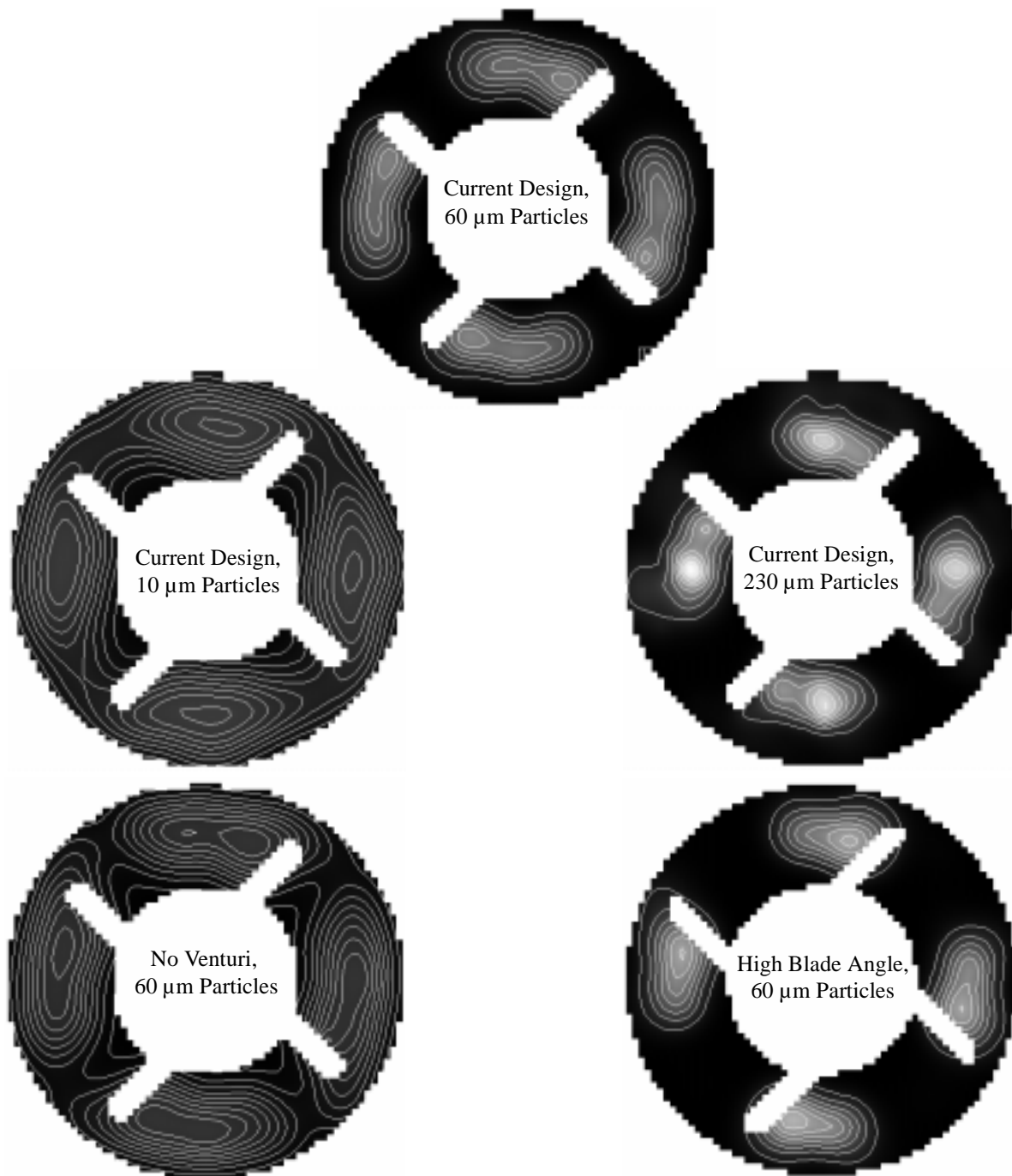


Figure 3. Particle mass density in the primary stream at the burner exit for various particle sizes and design configurations.

The 10 μ m particles, however, tend to be more uniformly distributed regardless of the flow field.

Simulations were also performed on the secondary and tertiary air streams. These simulations give useful quantitative information regarding the effectiveness of the vanes in imparting swirl to the flow at the burner exit plane and the spatial dependence of the velocity field due to the flow field boundaries (in particular, the effect of the presence of the leading edge of a flow-turning flare located slightly outside the

inner radius of the secondary stream). Qualitatively, the flow patterns predicted are not unexpected.

It is evident that any tangential gradients induced by the presence of the vanes have been damped out and that gradients in the axial velocity are in the radial direction ($U_{ax} = f_n \{r\}$). These radial gradients are quite large in the region near the flare leading edge and may serve as a flame anchor for this burner design. The velocity field in the tertiary stream is very similar to the outer portion of the secondary stream despite (1) a contraction that occurs approximately 6 inches from the burner exit and (2) the shorter distance from the swirl vanes to the burner exit. The swirl numbers predicted in the secondary and tertiary streams are also useful for comparison to simple predictions based on the vane angles (assuming no tangential momentum losses downstream of the vanes). For the secondary and tertiary streams (vanes at 30°) a simple prediction gives a tangential:axial velocity ratio of 0.577, while the detailed computational prediction based on integrated average velocity vectors at the exit plane gives 0.458 and 0.456 respectively. This could be significant in terms of effects on recirculation zones and inter-stream mixing in future furnace modeling.

Summary

- A model of char deactivation has been developed and verified illustrating that simple char oxidation models are inadequate for the prediction of carbon burnout in boilers, due primarily to the effects of thermal annealing.
- This burnout model, which has been adapted for future integration into a 3D, CFD-based reacting flow code, has been used to explain the low reactivity of residual carbon from boilers and can predict all of the significant features of the Sandia char combustion database.
- Modeling of the interior of a low- NO_x burner design has been used to illustrate the effects of design features (venturi, coal spreader blades) on particle distributions for a range of particles sizes and on the quantitative effectiveness of vanes as a means of imparting swirl in annular secondary flows. These results will be used as boundary conditions for future furnace models.

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