

# APPLICATION OF THE STOCHASTIC MODEL OF PARTICLE TURBULENT DISPERSION IN THE MODELING AND DESIGN OF A HIGH EFFICIENCY COAL COMBUSTOR

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## Introduction

In the modeling of pulverized coal combustion, the particle dispersion and transport in a turbulent flow are important issues. The accurate predictions of the flame structure and the radiation distribution rely strongly on how precisely the particle dispersion can be modeled. During the past decade, two major types of models have been developed: empirical and stochastic. In the empirical models by Lockwood et al. [1] and Smith et al. [2], the dispersion is assumed to be a diffusion process and is modeled by adding a diffusion velocity component to the mean particle velocity determined from the mean gas velocity. Empirical relations are used to calculate the diffusion velocity from the gas turbulence [1,2]. On the other hand, the stochastic models [3-5] treat particle motions in turbulence statistically. They trace the instantaneous interactions between particles and the turbulent eddies. Since the gas turbulence is stochastic in nature, these models are favored.

We have employed a stochastic model of particle dispersion in modeling a coal combustor for the design of a high temperature recuperative gas turbine topping cycle system [6]. The combustor contains a Radiatively Enhanced, Aerodynamically Cleaned Heat-Exchanger (REACH-Exchanger). The combustor is configured so that the working fluid is heated by the radiation from the coal flame while clean combustion gases are used to shield the ceramic heat exchanger tubes from the corrosive coal and ash particles. One of the important issues is to find the effect of various firing schemes on the particle dispersion, in order to prevent the ash particles from fouling the surface of the ceramic tubes.

In this paper, we present the further modification of the stochastic model and a few case studies showing how the firing scheme affects the particle dispersion. The combustion process is modeled by a 2D finite difference combustion code PCGC-2 [7].

## Stochastic Model

The particle motion is described in a Lagrangian framework as

$$\begin{cases} \frac{dU_i}{dt} = \Gamma(\bar{V}_i - U_i) + \Gamma V_i' + g_i \\ \frac{dX_i}{dt} = U_i \end{cases} \quad (1)$$

where  $U_i$  and  $V_i$  are the  $i^{\text{th}}$  ( $i=1,2,3$ ) components of velocity vectors of a particle and the gas, respectively;  $\Gamma$  accounts for the Stokes drag;  $X$  is the spatial coordinate of the particle;  $g_i$  is the gravity. Stochastic processes are specified with upper case characters and their realizations are given with

corresponding lower case characters. A prime indicates the fluctuation component of a stochastic process, and a bar indicates the mean value. In the stochastic model,  $V_i'$  is simulated with a random number generator. The particle is assumed to interact with eddies when it travels along with the gas stream. The gas velocity is assumed to be constant in each eddy. The length of the eddy is given by the length scale of the turbulence and the eddy decays with time according to the time scale. In other words, a particle sees a new eddy when it enters another eddy or the old one fades away. In the previous work [3,4,5],  $V_i'$  was generated directly by Monte Carlo methods and the interaction is handled in the numerical integration. A disadvantage of this method is that the results can be largely influenced by the numerical time step and it is not very efficient since the stochastic spectrum of the turbulence is not used. In this study, improvements of these early models were made based on the recent developments in the numerical integration of stochastic differential equations [8,9].

The stochastic characteristics of  $V_i$  are given by those of  $V_i'$  (turbulence model, k-ε) in terms of  $k$ ,  $l_0$ , and  $t_0$ , where  $k$  is the turbulence kinetic energy, and  $l_0$  and  $t_0$  are the length and time scales of the turbulence.  $V_i'$  is a stochastic process of both time,  $t$ , and distance,  $\mathbf{x}$ . The autocorrelation functions of  $t$  and  $\mathbf{x}$  are by definition

$$R_{V_i'}^t(\Delta t) = \exp(-|\Delta t|/t_0) \quad (2)$$

and

$$R_{V_i'}^x(\Delta \mathbf{x}) = \exp(-|\Delta \mathbf{x}|/l_0) \quad (3)$$

The double correlation is not readily available and is assumed to be

$$R_{V_i'}(\Delta \mathbf{x}, \Delta t) = \exp(-\sqrt{(\Delta t/t_0)^2 + (\Delta \mathbf{x}/l_0)^2}) \quad (4)$$

Since a particle sees the gas when it travels, the decay of the gas velocity seen by a particle traveling with velocity  $U$  is a function of  $\Delta t$  only. If  $R_{V_i'}$  decays quickly enough against  $\mathbf{x}$ , we have

$$R_{V_i',p}(\Delta t) = \exp(-\beta|\Delta t|) \quad (5)$$

where

$$\beta = \sqrt{(1/t_0)^2 + ((\bar{U}(\mathbf{x},t) - \bar{V}(\mathbf{x},t))/l_0)^2} \quad (6)$$

The second subscript  $p$  of  $R$  means that the correlation in Eq. (5) is for the gas seen by particles. From Eq. (5), we know that when seen by particles, the gas velocity fluctuation,  $V_i'$ , can be approximated with an Ornstein-Uhlenbeck process and can be generated with a filtered white noise [8]

$$\frac{dV_i'}{dt} = -\beta V_i' + \sigma_v \sqrt{2\beta} \xi_i(t) \quad (7)$$

where  $\sigma_v = (2/3k)^{0.5}$ .  $\xi_i(t)$  is a Gaussian white noise function. Or more formally

$$dV_i' = -\beta V_i' dt + \sigma_v \sqrt{2\beta} \Delta W_i(t) \quad (8)$$

where  $\Delta W_i(t)$  is an incremental Wiener process of Gaussian,  $N(0, \Delta t)$ . Since Eq. (8) contains explicitly  $\sigma_v$  and  $\beta$ , it can generate  $V_i'$  with correct gas turbulence statistics. We used differential equations (1) and (8) to model the particle dispersion by turbulence.

This set of equations is, however, intrinsically stiff for coal combustion problems, since very often the time scale,  $1/\beta$ , is much smaller than the particle relaxation time scale  $1/\Gamma$ . An implicit Euler scheme was employed in the integration to maintain the numerical stability.

## Case Studies

To investigate the effect of firing schemes on the coal particle dispersion, combustion in the REACH Reactor was modeled using various firing schemes. We present here only two of the cases studied. Table 1 lists the conditions of these two cases. The reactor is a 9 meter tall cylinder which is 2.8 meters in diameter. Coal particles were fired with the primary air at the center top position. Gas streams were injected from a number of annulus inlets. A schematic diagram of this reactor is given in Figure 1. The top view shows the relative positions of the inlets. The ceramic heat exchange tubes are located around the flame and next to the refractory wall, but they were not included in the calculations. The same mass flux of coal particles and air were used for both cases, except that there was a tertiary  $\text{CH}_4$ /air stream in Case 2. The diameter of the secondary air conduit in Case 1 was 1.27 meters, which was slightly larger than the 1.0 meters given in Figure 1 for Case 2.

The combustion was modeled with PCGC-2 [7] which provided the gas velocity and turbulence field information. The particle stochastic differential equations (1) and (8) were then solved. In each calculation, 100 particles were injected from 5 positions inside the primary tube and 100 particle trajectories were generated with our stochastic model. We used a PC based post-processor to visualize the results by injecting 5 particles every 0.08 second, so that a continuous particle stream was simulated. The particle diameter used in the calculation was 70  $\mu\text{m}$ .

### **Case 1**

Pulverized coal particles were down fired from a 0.39 meter diameter tube along with 15% of the combustion air. The secondary air which comprises the remainder of the total air entered through a 1.27 meter annulus. The vector plot of the mean gas velocity is shown in Figure 2a and the particle dispersion in Figure 2b. As expected, there was a large recirculation zone in the top part of the reactor. The positive radial velocity along with the turbulence caused a large scale particle dispersion in this case. Significant numbers of particles reached the refractory wall.

### **Case 2**

This case is displayed as a comparison to Case 1. Two additional inlets, secondary II and tertiary, were added in order to shield the ceramic heat exchanger tubes from the coal and ash particles. The tertiary gas stream was pre-mixed  $\text{CH}_4$  and air which entered through the outer annulus behind the heat exchanger tubes. To provide a buffer between the tubes and the flame, 2/3 of the secondary air was injected from secondary II and 1/3 of it entered from the secondary I. The secondary II inlet was approximately 0.25 meters in front of the heat exchanger tubes.

Figure 3a displays the gas flow pattern for this case and Figure 3b is the particle dispersion. The flow pattern obtained was considerably different from that obtained in Case 1 (Figure 2a). This is due to the added gas flux from the tertiary and the secondary II inlets. It demonstrates that firing schemes can effectively control the gas flow pattern. The particle dispersion near the wall region was much reduced in this case compared to Case 1. However, there were still a number of particles reaching the refractory wall at the bottom of the reactor.

## Discussions

The three major mechanisms of particle transport in a gas flow are transport by the background mean gas flow, turbulence dispersion, and the initial particle spray angle. The spray angle can be controlled by using converging and diverging nozzles. In this work, we have demonstrated that the gas flow pattern is controllable by employing special firing schemes. For the current geometry, we can effectively use the buffer air to provide some protection of the heat exchange tubes from the corrosive and erosive coal particles.

For Case 2, turbulence dominates the particle dispersion. Particle dispersion is then controlled by the shape and the position of the zone with high turbulence intensity. In combustion, it is closely related to the shape and the size of the flame. With the current axial symmetry geometry, this zone seems not to be affected significantly by the air flow and firing schemes. However, with an appropriately tailored reactor geometry, the shape of the turbulence zone can be controlled and the particle dispersion can be redirected. This concept is shown in Figure 4 with a rectangular shaped reactor. When the cleaning air inlets are added, the flame shape will be affected so that less particle turbulence dispersion will be directed toward the heat exchange tubes. Selecting an appropriate shape for the coal conduit can help to achieve the flame shape control.

In two other cases(not shown here), the effect of swirl in the secondary inlet was investigated. Results showed that swirl must be avoided in the REACH reactor since the tangential motion created by the swirl causes large scale particle dispersion.

For the REACH reactor, attention must also be paid to the radiative heat exchange from the combustion flame to the heat exchange tubes and the convective heat transfer from the tube wall to the working fluid [6]. In parallel to CFD modeling of the particle turbulence dispersion in the REACH reactor, experimental investigation of both the radiation heat transfer and the aerodynamic cleaning effect was performed and results will be published elsewhere [6].

#### **Acknowledgment**

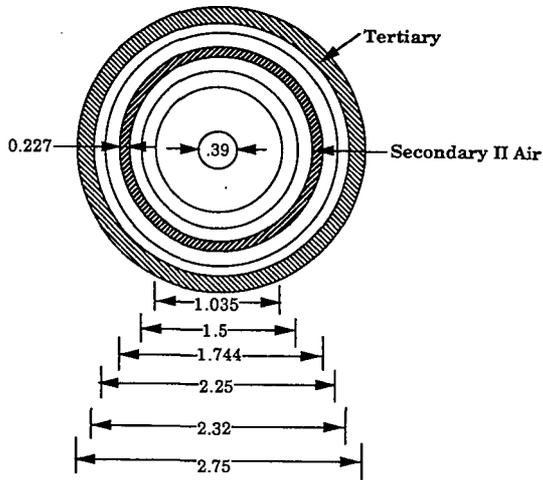
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Table 1. Flow conditions of Case 1 and 2.

		Flow Rates, Kg/s	
		Case 1	Case 2
Primary	Coal	0.50	0.50
	Air	0.88	0.88
Secondary I	Air	4.96	1.65
Secondary II	Air	-	3.31
Tertiary	CH <sub>4</sub>	-	0.067
	Air	-	1.34



Summary	
Primary Air and Coal	= 0.39 m
Secondary I Air	= 1.035 m
Secondary II Air	= 1.744 m
Flame	= 1.5 m
U-Tubes	= 2.25 m
Reactor	= 2.75 m

Figure 1. REACH-exchange reactor, Top View.

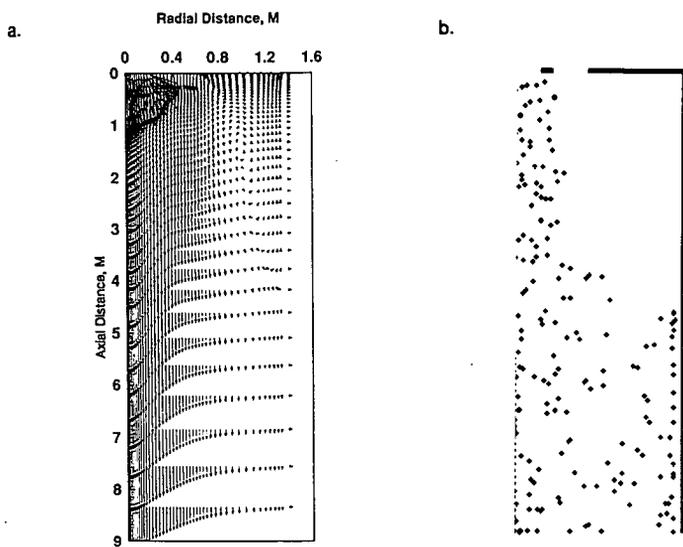


Figure 2. a. Velocity vector plot and b. particle dispersion of Case 1.

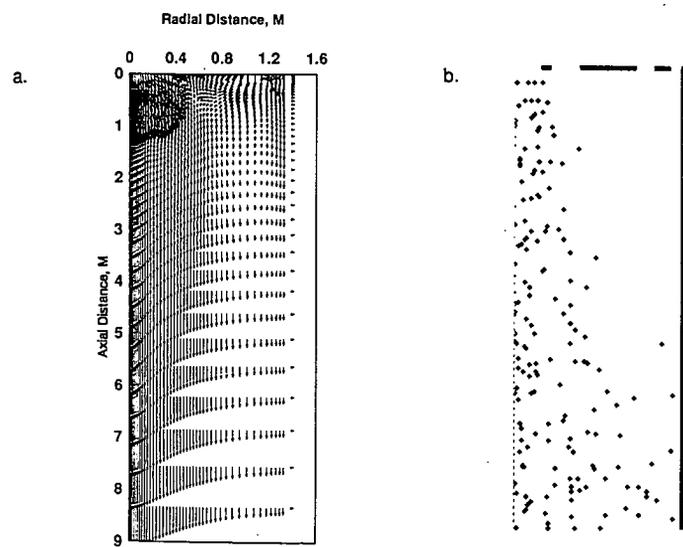


Figure 3. a. Velocity vector plot and b. particle dispersion of Case 2.

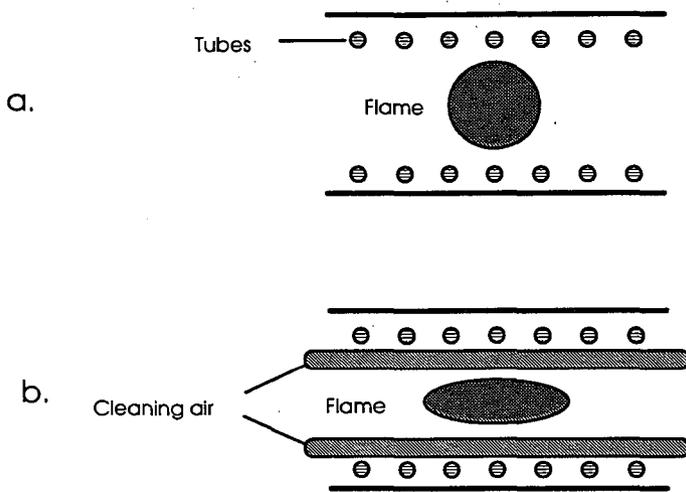


Figure 4. Top views of a rectangular REACH reactor, showing the effect of cleaning air on the shape of the flame. a. without the cleaning air and b. with the cleaning air.