RADIATION-TURBULENCE INTERACTIONS IN PULVERIZED-COAL FLAMES

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Preface

This is the Technical Report for the sixth quarter (second year, second quarter) of the project titled "Radiation-Turbulence Interactions in Pulverized-Coal Flames", which is funded by the Department of Energy, Pittsburgh Energy Technology Center (Grant #DE-FG22-93PC93210). The report covers the period from December 15, 1994 - March 30, 1995.

Two research associates, two Ph.D. students, and one M.S. student are involved in this project. Additional support for these researchers and the students has been received from a DOE Grant #DE-FG22-92PC533 (PI: M. P. Mengüç), from a NSF-EPSCoR Grant (PI: J.M. McDonough), and from the Department of Mechanical Engineering at UK.

Dr. Sivakumar Manickavasagam, a Research Associate, is primarily responsible for combining the fluid mechanics and radiative transfer computer codes. He is also in charge of developing a new algorithm to account for the soot agglomerate structure and char fragmentation. He and Dr. Sarbajit Ghosal, also a Research Associate, are responsible in designing the experimental system for future measurements.

Mr. Sudip Mukerji, a Ph.D. student, is developing the computer codes for simulation of turbulence using the additive turbulent decomposition (ATD) technique in two and three dimensional geometries. Mr. Derong Wang, another Ph.D. student is primarily supported by a NSF/EPSCoR project. He is modeling the interaction of radiation beam with small scale ATD technique.

Mr. Ramaswamy Govindan is a M.S. student. He has worked on a model to couple radiation turbulence interactions in our flames. In addition to that, he is developing a new optical system to identify particle properties from their polarized scattering characteristics. He is supported mainly by the DOE Grant #DE-FG22-92PC533 and the Department of Mechanical Engineering.

During this period, experiments are carried out and preliminary data were collected. Also, a paper on fractal type soot agglomerates has been prepared. We are going to report on both of these accomplishments in the next report as more details will be ready.

Here, we are submitting a copy of our paper accepted for presentation at the First

International Symposium on Radiative Transfer, which will be held in Kusadasi, Turkey, in August 1995.

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RADIATION-TURBULENCE INTERACTION IN FLAMES USING ADDITIVE TURBULENT DECOMPOSITION

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ABSTRACT: The purpose of this paper is to discuss the nature of the unsteady interactions between buoyant turbulence and radiation feedback to the center of flames. An unfiltered additive turbulent decomposition (ATD) is carried out in a manner similar to that originally developed by McDonough and co-workers for studying Burgers' equation. The new approach is philosophically similar to LES; namely, treat the large and small scales separately. However, the technique requires no formal filtering or averaging for the large-scale equations, and the corresponding subgrid-scale models are obtained as local spectral approximations of the original governing equations. In the present work, only the small-scale part of the governing equations has been solved, and the large-scale parameters are to be obtained directly from either a global computer program or from corresponding experimental results. Preliminarily calculated results show that the radiation in the flame markedly influences the flow in the center of flame, and even periodic radiation fluctuations can lead to chaotic behavior of the flow. The extent to which the flow fluctuates not only depends on fluctuation of radiative properties, but also on the profile of the mean absorption coefficient.

1. INTRODUCTION

1.1. Background

Several complicated phenomena occur simultaneously in combustion systems, including turbulent fluid flow, heat transfer, radiation, chemical kinetics, and phase change leading to pollution formation, ash deposition, etc. Among all these phenomena, probably radiation transfer and turbulence deserve special recognition, as their interaction has never been studied in coal flames.

Radiation transfer accounts for as much as 90% of the total heat transfer to the refractories of large-scale pulverized-coal fired furnaces. Although the accuracy of radiative transfer

models has improved steadily during the last decade, still we are far from being able to predict radiative flux and source terms with very good accuracy, mainly because of the lack of information on spectral particle properties and volume concentration distributions (Viskanta and Mengüç, 1987; Mengüç and Webb, 1993). At the same time, it is very important to understand the fundamentals of turbulent reacting flow fields, as the flames in virtually all industrial furnaces are turbulent in nature (McMurtry and Queiroz, 1993). Unfortunately, the widely employed turbulence models in practical systems, such as the $k-\epsilon$ model, are far from being physically realistic and cannot be used to study the underlying physical phenomena yet to be discovered.

Further fundamental research both on radiative transfer and turbulence need to be carried out to improve the efficiency and economy of combustion systems. Yet, what we emphasize in this paper is neither of these areas separately, but their *interaction*.

The attempts to account for the effects of radiation on flow and temperature fields in a turbulent environment include those by Cox (1977), Tamanini (1977), Kabashnikov and Kmit (1979), Grosshandler and Joulain (1986), Fischer et al. (1987), Fischer and Grosshandler (1988), as well as Faeth and his students (Gore and Faeth, 1986, 1988; Gore et al., 1987a and 1987b, Kounalakis et al., 1988 and 1991; Gore, 1988) who discussed and showed the strong coupling effects between turbulence and radiation. A detailed discussion of studies related to radiation-turbulence interactions was given by Faeth et al. (1985, 1989).

Although several significant advances have been made in understanding the radiation-turbulence interactions in gaseous flames (especially by Faeth and his co-workers), we are still not capable of predicting these fundamental interactions starting from first principles. There is a definite need to employ more sophisticated turbulence simulation techniques along with accurate and reliable radiation and chemical kinetics models to develop a thorough understanding of these complex phenomena and their interactions.

In most flames studied in the literature, combustion gases H_2O and CO_2 are the only participants in radiation absorption and emission. But the gas contribution becomes secondary if there are particles present, such as soot; the reason for this stems from the spectral nature of radiative transfer. Gases emit and absorb at certain wavelengths, or frequencies, which are related to vibrational-rotational interactions of diatomic molecules. On the other hand, soot particles absorb and emit in continuum, i.e., over the entire wavelength spectrum. Given this, it becomes obvious that any external effects, such as turbulent fluctuations, are likely to have a larger impact if soot is present (even without considering possible hydrodynamic effects of soot). Indeed, the preliminary calculations show that unless the effects of fluctuations are accounted for, the radiative source term is significantly underpredicted by more than 50%. The importance of this error can be realized by noting that the radiation source term is the major contributor to the balance of energy in coal-flames; without having it accounted for accurately, the local temperatures cannot be determined with confidence. Errors in temperature

then yield wrong predictions about the local chemistry, coal devolatilization, pyrolysis, and soot yield, which affect the predictions about the performance of the combustion chambers. Therefore, without having a fundamental understanding of radiation-turbulence interactions, it is not possible to claim that efficient and environmentally acceptable design of furnaces would be realized.

1.2. Objectives

We are going to present a detailed mathematical analysis for a simple physical system to understand the extend of radiation-turbulence interaction. Turbulence simulations will be carried out using the additive turbulent decomposition approach. Chaotic and periodic maps will be used to model the fluctuations of properties in a simple triangular-shaped flame. Radiation contributions will be accounted for by considering detailed line-of-sight integrations.

2. ANALYSIS

In this section we will introduce the additive turbulent decomposition formalism in a general context, present the governing equations of our model problem, apply ATD to these and describe the numerical implementation, and finally give some details of the governing equations for radiation transfer.

We wish to stress at the outset that we will employ the term “turbulence model” to mean some set of equations that may, or may not, be consistent with the Navier-Stokes (N.-S.) equations and which effects closure of a system that has more unknowns than the number of equations. Similarly, the terminology “turbulence simulation” will be associated with methods that are closed, and for which no modeling is needed.

2.1. Additive Turbulent Decomposition Formalism

In this subsection we will provide a brief overview of the conceptual underpinnings of ATD. McDonough et al. (1984a,b) considered a new approach to turbulence simulation that originally was termed “large-scale/small-scale decomposition.” Features of this technique included: i) unaveraged equations, thus avoiding the turbulence closure problem, ii) complete consistency with the N.-S. equations, and iii) high degree of parallelizability. The method has been developed by McDonough and Bywater (1986, 1989a) in the context of Burgers’

equation, by Hylin and McDonough (1991) and Yang and McDonough (1992) for 2-D incompressible N.-S. equations, by McDonough and Saito (1995) for 1-D compressible N.-S. with simple chemistry, and McDonough and Wang (1995) have studied the parallelization of the small-scale equations.

The basic steps in constructing the ATD algorithm are as follows. First, decompose dependent variables into large- and small-scale parts, as would be done in LES. Second, additively decompose the governing equations into large-scale and small-scale equations. We note that this second step leads to the same equations as obtained by Marion and Temam (1989) in nonlinear Galerkin methods, but the solution procedure we employ is more general. Finally, we spatially decompose the small-scale equation in a manner completely analogous to domain decomposition methods (cf. Glowinski et al., 1988). It is this step that leads to the high degree of parallelizability of ATD.

To make these discussions more concrete we will consider the vector equation,

$$q_t + \nabla \cdot F(q) + \nabla \cdot (D(q)\nabla q) = S(q), \quad (1)$$

to be solved on some domain $\Omega \subset \mathbf{R}^3$ with initial conditions defined on Ω and boundary conditions prescribed on $\partial\Omega$. We note that this form is sufficiently general to include essentially any transport equation, and in particular, the nonlinear source term $S(q)$ will provide direct coupling of radiation effects to the hydrodynamics via the thermal energy equation.

The first step in applying ATD to Eq.(1) is to decompose the dependent variables into large-scale and small-scale parts in a manner similar to what is done in Reynolds-averaged approaches, and in LES:

$$q(x, t) = \bar{q}(x, t) + q^*(x, t), \quad x \in \Omega. \quad (2)$$

Here, $\bar{q}$ should be viewed as the first terms in a Fourier representation of q , and q^* is the remainder. This interpretation is very different from that of classical Reynolds averaging, but it is actually equivalent to LES. In the second step we substitute Eq.(2) into Eq.(1) and additively decompose the result in a manner quite analogous to typical locally one-dimensional (LOD) time splitting (cf. Mitchell and Griffiths, 1980). This leads to the coupled system of vector equations for $\bar{q}$ and q^* :

$$\frac{\partial \bar{q}}{\partial t} + \nabla \cdot \left[F(\bar{q}) + \frac{A}{2} F(\bar{q}, q^*) \right] + \nabla \cdot \left[\left(D(\bar{q}) + \frac{B}{2} D(\bar{q}, q^*) \right) \nabla \bar{q} \right] = S(\bar{q}) + \frac{C}{2} S(\bar{q}, q^*) \quad (3)$$

$$\frac{\partial q^*}{\partial t} + \nabla \cdot \left[F(q^*) + \frac{A}{2} F(\bar{q}, q^*) \right] + \nabla \cdot \left[\left(D(q^*) + \frac{B}{2} D(\bar{q}, q^*) \right) \nabla q^* \right] = S(q^*) + \frac{C}{2} S(\bar{q}, q^*) \quad (4)$$

These equations are exact for polynomial nonlinearities, but must be augmented with use of quasilinearization for genuine nonlinearities such as arise from Arrhenius chemical kinetics.

An important observation is that there is no closure problem associated with Eqs.(3) and (4); the number of equations equals the number of unknowns. Moreover, it is not difficult to show that discrete approximations to the solution of Eqs.(3) and (4) are equivalent, up to the lowest order of discretization, to the discrete approximations of Eq.(1). In fact, McDonough et al. (1989) have shown this to be true for the incompressible N.-S. equations even without iteration between Eqs.(3) and (4) provided a certain predictor-corrector algorithm is employed. Thus, this system is consistent with the N.-S. equations and is equivalent to DNS. However, for problems of the complexity to be considered in the present study, far too much arithmetic would be required to permit such calculations in 3-D, even though the small-scale equations Eq.(4) can be implemented in a highly parallelizable fashion. Consequently, we will focus attention on very small, local regions of the flow field, and solve only the small-scale equations. This is similar to minimal DNS (Moin, 1992) except that unlike minimal DNS, our small-scale equations explicitly contain large-scale quantities. Their presence allows direct account to be taken of local large-scale (integral-scale) flow behavior and thus reduces the number of modes (or grid points) needed to achieve resolution all the way to the dissipation scales. Yang and McDonough (1992) have shown that even at quite high Reynolds number Re (up to $O(10^6)$), as few as seven Fourier modes in each spatial direction provide adequate resolution to capture qualitative features of the flow field. The disadvantage of the approach is that the large-scale quantities appearing in Eq.(4) must be obtained in some independent, and obviously approximate, way.

2.2. Governing Equations

The 1-D continuity, momentum, and energy equations for flow along the axis of a diffusion flame can be written as:

$$\rho_t + (\rho u)_x = 0 \quad (5)$$

$$\rho u_t + \rho u u_x = \rho \beta g (T - T_0) + \mu u_{xx}, \quad (6)$$

$$\rho C_p T_t + \rho C_p u T_x = k T_{xx} - \nabla \cdot q_r. \quad (7)$$

Here, ρ is density, u is upward (x -direction) velocity, T is temperature, μ is viscosity, k is heat conductivity, β is the coefficient of thermal volumetric expansion, g is acceleration of gravity, C_p is specific heat capacity, and T_0 is the ambient temperature. The Boussinesq approximation is introduced in the momentum equation to handle effects of buoyancy, and in the energy equation the radiation emitted from the assumed flame sheet is included as the source term at the centerline; i.e., q_r is the radiative heat flux. We will employ these equations with the following radiation model to study radiation-turbulence interactions along the axis of a flame.

At any point A along the axis of the flame depicted in Figure 1, the radiation heat flux can be written as:

Figure 1. One-dimensional flame model

$$\nabla \cdot q_r = \kappa(4\sigma T^4 - G). \quad (8)$$

Here the flame is assumed to be gray, although this will be modified later; κ is absorption coefficient, and σ is the Stefan-Boltzmann constant. If it is assumed that the temperature at the center of the flame is much lower than that of the flame sheet, the heat flux can be expressed as

$$\nabla \cdot q_r = -\kappa G, \quad (9)$$

where G is the incident radiation at point A, which can be calculated from:

$$G = \int_{\Omega=4\pi} I_A(\Omega) d\Omega. \quad (10)$$

Intensity I_A can be determined from the solution of the integral form of the radiation transfer equation, which can be written along an Ω direction as

$$I_A(\Omega) = \int_0^{\tau_s} \frac{\sigma T_f^4(\tau_{s'})}{\pi} \exp(\tau_s - \tau_{s'}) d\tau_{s'}, \quad (11)$$

where

$$\tau_s = \int_0^s \kappa(s') ds' \quad (12)$$

is the optical thickness over a distance s . Note that we are not using any particular model for the radiative transfer. The incident radiation will be determined by approximating the integral, Eq. (11), using a finite number of different directions.

The dimensionless form of Eqs. (5-7) can now be written as:

$$\rho_t + (\rho u)_x = 0, \quad (13)$$

$$\rho u_t + \rho u u_x = \frac{Gr}{Re^2} \rho T + \frac{1}{Re} u_{xx}, \quad (14)$$

$$\rho T_t + \rho u T_x = \frac{1}{Re Pr} T_{xx} + N_R G, \quad (15)$$

where Re, Pr, Gr are the usual Reynolds, Prandtl and Grashof numbers, respectively. The radiation parameter N_R is defined as

$$N_R = \frac{\tau_L \sigma T_s^4}{\rho C_p U_0 (T_s - T_0)}, \quad (16)$$

where

$$\tau_L = \int_0^L \kappa dx. \quad (17)$$

2.3. Application of ATD

Application of additive turbulent decomposition to Eqs. (5-7) begins by decomposing dependent variables in the manner indicated in Eq. (2); namely,

$$\rho = \bar{\rho} + \rho^*, \quad u = \bar{u} + u^*, \quad T = \bar{T} + T^*. \quad (18)$$

Equations (18) are substituted into Eqs. (13-15), and the result decomposed additively (essentially a Hilbert space decomposition into subspaces) to obtain the specific forms corresponding to Eqs. (3,4).

Large-scale equations:

$$\bar{\rho}_t + (\bar{\rho} \bar{u})_x + \frac{1}{2} (\bar{\rho} u^* + \rho^* \bar{u})_x = 0 \quad (19)$$

$$\rho \bar{u}_t + \rho \bar{u} \bar{u}_x + \frac{1}{2} \rho (\bar{u} u_x^* + u^* \bar{u}_x) = \frac{Gr}{Re^2} \rho \bar{T} + \frac{1}{Re} \bar{u}_{xx} \quad (20)$$

$$\rho \bar{T}_t + \rho \bar{u} \bar{T}_x + \frac{1}{2} \rho (\bar{u} T_x^* + u^* \bar{T}_x) = \frac{1}{Re Pr} \bar{T}_{xx} + N_R \bar{G}. \quad (21)$$

Small-scale equations:

$$\rho_t^* + (\rho^* u^*)_x + \frac{1}{2} (\bar{\rho} u^* + \rho^* \bar{u})_x = 0 \quad (22)$$

$$\rho u_t^* + \rho u^* u_x^* + \frac{1}{2} \rho (\bar{u} u_x^* + u^* \bar{u}_x) = \frac{Gr}{Re^2} \rho T^* + \frac{1}{Re} u_{xx}^* \quad (23)$$

$$\rho T_t^* + \rho u^* T_x^* + \frac{1}{2} \rho (\bar{u} T_x^* + u^* \bar{T}_x) = \frac{1}{Re Pr} T_{xx}^* + N_R G^*, \quad (24)$$

where

$$\bar{G} = \int_{4\pi} \bar{I}_A d\Omega, \quad (25)$$

and

$$G^* = \int_{4\pi} I_A^* d\Omega, \quad (26)$$

with

$$\bar{I}_A = \int_0^{\tau_s} \frac{4}{\pi} (\bar{T}_f^4 + f(\bar{T}_f, T_f^*)) \exp(\tau_s - \tau_{s'}) d\tau_{s'}, \quad (27)$$

$$I_A^* = \int_0^{\tau_s} \frac{4}{\pi} (T_f^{*4} + f(\bar{T}_f, T_f^*)) \exp(\tau_s - \tau_{s'}) d\tau_{s'}, \quad (28)$$

$$f(\bar{T}_f, T_f^*) = 2\bar{T}_f^3 T_f^* + 6\bar{T}_f^2 T_f^{*2} + 2\bar{T}_f T_f^{*3}. \quad (29)$$

Here, $\bar{T}_f$ and T_f^* are, respectively, the large- and small-scale parts of the flame temperature.

2.4. Numerical Implementation

The large-scale equations (19-21) and the small-scale equations (22-24) can in general be solved with different methods, permitting the tailoring of the method for the required level of resolution. In this study we will not solve the large-scale equations, and we solve the small-scale equations only locally (an advantage of ATD) to facilitate investigation of flame instabilities at specific points along the flame axis.

The basic approach is to consider these equations locally on subintervals of length $O(h)$, where h is the large-scale discretization stepsize, and construct local Galerkin approximations

for dependent variables on each such subinterval. On each local subinterval the dependent variables can be expressed in the form

$$\rho^*(x, t) = \sum_{k=1}^K a_k(t) \sin(\sigma_{kh} x^*), \quad (30)$$

$$u^*(x, t) = \sum_{k=1}^K b_k(t) \cos(\sigma_{kh} x^*), \quad (31)$$

$$T^*(x, t) = \sum_{k=1}^K c_k(t) \sin(\sigma_{kh} x^*), \quad (32)$$

where $\sigma_{kh} = \frac{k\pi}{h}$, and $x^* = x - (x_i - \frac{h}{2})$, with $x \in [x_i - \frac{h}{2}, x_i + \frac{h}{2}] \equiv \Omega_i^h$.

Substituting Eqs. (30-32) into (22-24) and forming the Galerkin inner products in the usual manner leads to a system of ordinary differential equations (ODEs) for the time-dependent Fourier coefficients:

$$\dot{a}_k(t) = C_0 \frac{\pi}{h} \sum_{l,m}^K a_m b_l (l A_{klm} - m B_{lmk}) - \frac{1}{2} C_0 \sum_l^K (\bar{\rho}_x b_l S_{kl} - \frac{\pi}{h} \bar{u} l a_l S_{kl}) + \frac{1}{2} (\frac{k\pi}{h} \bar{\rho} b_k - \bar{u}_x a_k), \quad (33)$$

$$\dot{b}_k(t) = C_0 \frac{\pi}{h} \sum_{l,m}^K l b_m b_l B_{klm} + \frac{C_0 \pi \bar{u}}{2h} \sum_l^K l b_l S_{lk} + C_0 \frac{Gr}{Re^2} \sum_l^K c_l S_{kl} - \frac{1}{2} \bar{u}_x b_k - \frac{k^2 \pi^2}{\rho Re h^2} b_k, \quad (34)$$

$$\dot{c}_k(t) = -C_0 \frac{\pi}{h} \sum_{l,m}^K l c_l b_m B_{lmk} - \frac{C_0 \pi \bar{u}}{2h} \sum_l^K l c_l S_{kl} - \frac{1}{2} C_0 \bar{T}_x \sum_l^K b_l S_{kl} - \frac{1}{\rho Re Pr} \frac{k^2 \pi^2}{h^2} c_k + \frac{N_R}{\rho} G_k^*, \quad (35)$$

where $G_k^* = \frac{h}{k\pi} [1 - (-1)^k] G^*$. Here Heun's method (a second-order Runge-Kutta) is employed to solve this system with constant dimensionless time step $\Delta t = 5 \times 10^{-6}$ continued for 20000 time steps. The coefficients used in these equations are defined as:

$$C_0 = \left(\int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} \sin^2 \sigma_{kh} x^* dx \right)^{-1} = \frac{2}{h}$$

$$S_{kl} = \int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} \sin \sigma_{kh} x^* \cos \sigma_{lh} x^* dx = \begin{cases} \frac{h}{2\pi} (\frac{1}{k+l} + \frac{1}{k-l}) & \text{if } \text{mod}(k+l, 2) \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} A_{klm} &= \int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} \sin \sigma_{kh} x^* \sin \sigma_{lh} x^* \sin \sigma_{mh} x^* dx \\ &= \begin{cases} \frac{h}{4\pi} (\frac{1}{k-l+m} + \frac{1}{k-l-m} + \frac{1}{k+l+m} + \frac{1}{k+l-m}) & \text{if } \text{mod}(k+l+m, 2) \neq 0 \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

$$\begin{aligned}
B_{klm} &= \int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} \cos \sigma_{kh} x^* \sin \sigma_{lh} x^* \cos \sigma_{mh} x^* dx \\
&= \begin{cases} \frac{h}{4\pi} \left(\frac{-1}{k-l+m} - \frac{1}{k-l-m} + \frac{1}{k+l+m} + \frac{1}{k+l-m} \right) & \text{if } \text{mod}(k+l+m, 2) \neq 0 \\ 0 & \text{otherwise} \end{cases}
\end{aligned}$$

$$D_{klm} = \int_{x_i - \frac{h}{2}}^{x_i + \frac{h}{2}} \sin \sigma_{kh} x^* \cos \sigma_{lh} x^* \sin \sigma_{mh} x^* dx = \begin{cases} \frac{h}{8\pi} & \text{if } k = l + m \text{ or } k = l - m \\ \frac{-h}{8\pi} & \text{if } k = m - l \\ 0 & \text{otherwise} \end{cases}$$

2.5. Calculation of Incident Small-Scale Radiation G^*

To simplify the problem, the flame shape is assumed to be conical as indicated in Fig. 1. Therefore the intensity at the center of the flame is a function of θ , but is independent of azimuthal angle. Then

$$G^* = 2\pi \int_0^\pi I_A^*(\theta) \sin(\theta) d\theta. \quad (36)$$

The temperature in the flame and radiation absorption coefficient are considered to be fluctuating, and T_f^* and κ^* are modeled by a modified logistic map formulated as follows:

$$M^{(n+1)} = CM^{(n)}(1 - |M^{(n)}|). \quad (37)$$

M is a map value which fluctuates between approximately -1.2 and 1.2 . At $C = 4.82$, a chaotic time series will be generated. To calculate κ^* and T_f^* at each time step n , we use the following formulas

$$\kappa^* = \kappa M(n), \quad (38)$$

$$T_f^* = \bar{T} M(n), \quad (39)$$

where κ and $\bar{T}$ are local absorption coefficient and temperature, respectively. It is assumed here that the profiles for κ and $\bar{T}$ in the conical flame are available and given as:

$$\kappa = \kappa_0 \left(\frac{x}{L} + 0.2 \right) \exp[-2(1 - \frac{r}{R})], \quad (40)$$

$$T = T_{fl} \left(\frac{x}{L} + 0.4 \right) \exp[-0.5(1 - \frac{r}{R})]. \quad (41)$$

where κ_0 and T_{fl} are assumed as absorption coefficient and temperature on flame sheet, respectively. Note that the initial seed of the map is assigned locally at each computational point in the flame via the chaotic map (Eq. 37). In addition, incident radiation G^* is calculated at each time step by trapezoidal quadrature (step size $\Delta h = 0.01$). We should observe here that this use of nonlinear algebraic maps as models of fluctuating flame temperature and absorptivity represents a very simplistic version of the ATD modeling approach introduced in McDonough et al. (1995) for turbulent fluid flow.

3. RESULTS AND DISCUSSION

In this section we will present sample calculated results obtained from the model discussed above. All computations were performed on the Convex-HP Exemplar at the University of Kentucky Computer Center (UKCC) using software written in double precision FORTRAN 77.

Since our primary aim in the present work is to describe the qualitative aspects of unstable behavior in flames, only the small-scale equations are solved. All large-scale quantities are to be obtained from either a global computer program or from experimental data. Flame height is taken as $L = 1m$. The temperature (T_{fl}) on the flame sheet is assumed as $2000K$ and the corresponding absorption coefficient (κ_0) is taken as $200m^{-1}$ or $300m^{-1}$ in order to investigate its influence on flow. The small-scale equations were solved at $x = 0.90$, where x is dimensionless height. The calculations employed an effective large-scale finite difference grid spacing $h = 5 \times 10^{-4}$, and the number of Fourier modes was $K = 15$. The results reported here were calculated for $Re = 10^5$ and $Gr = 10^{13}$. The maximum amplitude of the absorption coefficient and flame temperature fluctuations is assumed as 50% of κ_0 and T_{fl} .

Figure 2a shows the time series of small-scale velocity when no radiation interaction is occurring. Figure 2b is its corresponding power spectral density (psd). The combination of time series and psd can often provide sufficient information to determine the underlying dynamics of the system that generated the time series. Periodic behavior is usually obvious from the time series, itself, while the psd quantifies this in terms of squared amplitude (appropriately scaled, usually as decibels, db) of corresponding Fourier coefficients vs. frequency. A sharp peak occurs in the psd for each frequency (or harmonic, or subharmonic) present in the signal. Quasiperiodicity may, or may not, be obvious from the time series, but it is relatively easy to recognize in the psd. In particular, it appears as two, or more, dominant peaks occurring at non-integrally related (incommensurate) frequencies, along with their various harmonics. Chaotic behavior cannot necessarily be determined from time series and psds alone, but often these provide a strong indication. If the time series appears aperiodic, then it will be either chaotic or random. In the former case, the psd will be broad-band, but will typically (but not always) exhibit $f^{-\alpha}$ ($\alpha \geq 1$) decay. The psd of a random signal is

usually "white", i.e., all frequencies occur at essentially equal power. From Figs. 2a,b we can see that the flow evidently behaves quasiperiodically. In order to account for the radiation contribution, we employ a periodic map (see Fig. 2c,d) and a chaotical map (Figure 2g,h) to represent the small-scale absorption coefficient and temperature fluctuations. Figure 2e gives the calculated time series of velocity in the case of periodic radiation fluctuations, and Fig. 2f is its power spectral density. Figures 2i and 2j are the calculated results for the case of chaotic radiation fluctuations. These figures show that both periodic and chaotic radiation fluctuations can generate chaotic flow.

This is not surprising because the base flow is quasiperiodic, and it is known from Ruelle and Takens (1971) that such flows are unstable in the sense that chaotic attractors lie arbitrarily close to them; hence, any small perturbation may trigger a transition from the quasiperiodic state to the chaos of a strange attractor. On the other hand, details of the two resulting chaotic flows are rather different. In the particular, it is evident that the one resulting from periodic forcing retains the forcing period along with its broad-band behavior (Fig. 2f), while that arising from chaotic forcing is purely broad-band (Fig. 2j), even though the forcing amplitudes are essentially the same. Moreover, the amplitude of small-scale velocity fluctuations arising from the periodic map is smaller than that of the chaotic map. This tells us that the extent of fluctuation of radiation in the flame directly influences the flow field in the center of flame. In addition, we can see that even though the psd for chaotic radiation fluctuations themselves does not decay, that corresponding to the calculated velocity does decay because of the dissipative effects of viscous and thermal diffusion in the Navier-Stokes and energy equations.

Figures 3 and 4 display the time series of calculated small-scale velocity and temperature, respectively, in four different cases, corresponding to no radiation, periodic absorption coefficient, and two different amplitudes of chaotic absorption coefficient. We can see that the qualitative nature of the chaotic radiation fluctuations strongly affects the maximum extent to which the flow behaves chaotically. It can also be seen that the amplitude of the average absorption coefficient plays a very important role in the radiation-turbulence interactions. From Fig. 3 we see that the mean amplitude of the small-scale velocity is slightly lower in the presence of radiation, and that this mean amplitude is relatively insensitive to either the type or amplitude of the absorption coefficient fluctuations. At the same time, the fluctuations about this mean amplitude are quite sensitive to the type and level of absorption coefficient fluctuation.

Figure 4 shows that the effects on small-scale temperature are somewhat different in detail. It does not appear that the mean (small-scale) temperature is significantly affected by the periodic absorption coefficient fluctuations, although it appears to shift slightly downward with increasing magnitude of the chaotic forcing. But just as observed in Fig. 3 for small-scale velocities, fluctuations about the mean are strongly influenced by the type and magnitude

of absorption coefficient. For both velocity and temperature, increasing the degree of chaos in absorption coefficient results in increasing amplitude fluctuations about the small-scale mean.

4. SUMMARY AND CONCLUSIONS

In this paper we have discussed the importance of considering the interaction between radiation and turbulence, and we provided a brief review of current literature to indicate the difficulty (impossibility?) of doing this in detail with any of the standard approaches currently used for turbulence calculations. We then introduced the additive turbulent decomposition formalism and treated a 1-D model problem corresponding to a buoyant diffusion flame to demonstrate the potential of this method for simulating radiation-turbulence interactions.

The results obtained from this model problem are very encouraging. Although one must always beware of making general statements about fluid flow based on 1-D simplified model results, we should also recognize that the small-scale equations we have treated here comprise a nonlinear dynamical system, independent of the number of spatial dimensions present in the problem from which they have been derived, and that such systems tend to exhibit rather generic behaviors.

In light of this, we somewhat cautiously conclude the following: By means of the ability afforded by ATD to accurately focus on small computational regions while retaining local large-scale influences, we have been able to demonstrate qualitative effects of radiation on the flow field along the axis of our model diffusion flame. We accomplished this by comparing cases with no radiation with several cases of fluctuating absorption coefficient and finding that there is a transition from quasiperiodic (no radiation) to chaotic behavior in the presence of radiation. Although we have not yet completely quantified this chaotic behavior, what we can conclude is that fluctuation amplitudes about the small-scale mean increase significantly for both centerline velocity and temperature as the absorption coefficient fluctuation amplitudes are increased. This appears to be in accord with what one would expect on physical grounds, and provides a motivation for more thorough study of application of ATD to the radiation-turbulence interaction problem.

(a)

(b)

(c)

(d)

(e)

(f)

Figure 2. Time series (left-side panels) and their corresponding power spectral density (right-side panels)

(a) (b) small-scale velocity without radiation

(c) (d) periodic map (sine function)

(e) (f) small-scale velocity with periodic radiation forcing

Figure 2 (Cont.)

(g) (h) chaotic map

(i) (j) small-scale velocity with chaotic radiation forcing

(a)

(b)

(c)

(d)

Figure 3. Time series of small-scale velocity

(a) without radiation

(b) with periodic radiation forcing (absorption coeff. = $200(m^{-1})$)

(c) with chaotic radiation forcing (absorption coeff. = $200(m^{-1})$)

(d) with chaotic radiation forcing (absorption coeff. = $300(m^{-1})$)

(a)

(b)

(c)

(d)

Figure 4. Time series of small-scale temperature

- (a) without radiation
- (b) with periodic radiation forcing (absorption coeff. = $200(m^{-1})$)
- (c) with chaotic radiation forcing (absorption coeff. = $200(m^{-1})$)
- (d) with chaotic radiation forcing (absorption coeff. = $300(m^{-1})$)

Figure 4. Time series of small-scale temperature

- (a) without radiation
- (b) with periodic radiation forcing (absorption coeff. = $200(m^{-1})$)
- (c) with chaotic radiation forcing (absorption coeff. = $200(m^{-1})$)
- (d) with chaotic radiation forcing (absorption coeff. = $300(m^{-1})$)

5. REFERENCES

- Cox, G. (1977), *Combust. Sci. and Tech.*, Vol. 17, pp. 75-78.
- Faeth, G.M., Jeng, S.M., and Gore, J., (1985), *Heat Transfer in Fire and Combustion Systems*, Edited by C.K. Law, Y. Jaluria, W.W. Yuen, K. Miyasaka, HTD-Vol.45, pp.137-151.
- Faeth, G.M., Gore J.P., Chuech, S.G. and Jeng, S.M., (1989) *Ann. Rev. Numerical Fluid Mech. and Heat Transfer* C.L. Tien and T.C. Chawla, eds. Hemisphere, New York, pp. 1-38.

Fischer, S.J., Hardouin-Duparc, B. and Grosshandler, W.L., (1987), *Comb. Flame*, Vol 70, pp. 291-306.

Fischer, S.J. and Grosshandler, W.L., (1988), *Twenty-Second Symposium (International) on Combustion*. The Combustion Institute, Pittsburgh, PA, 1241-1250.

Glowinski, R. Golub, G. H., Meurant, G. A. and Periaux, J., (1988). *Domain Decomposition Methods for Partial Differential Equations*, SIAM, Philadelphia.

Gore, J.P., (1988), *Collected Papers in Heat Transfer 1988*, Vol. 2 (K.T. Yang, ed.), ASME, New York, pp. 77-86.

Gore, J.P. and Faeth G.M. (1986), *Twenty-First Symposium (International) on Combustion*. The Combustion Institute, Pittsburgh, PA, pp. 1521-1531.

Gore, J.P., Jeng, S.M. and Faeth, G.M. (1987a), *AIAA J.* Vol. 25, No. 2 pp. 339-345.

Gore, J.P., Jeng, S.M. and Faeth, G.M. (1987b), *J. Heat Trans.*, Vol. 109, No. 1, pp. 165-171.

Gore J.P. and Faeth G.M. (1988), *J. Heat Trans.*, Vol. 110, No. 1, pp. 173-181.

Grosshandler, W.L. and Joulain, P. (1986), *Prog. Astro. and Aero.*, Vol. 105, Part II, AIAA, Washington, pp. 123-152.

Hylin, E. C. and McDonough, J. M., (1991), *4th Int. Sympos. on Computational Fluid Dynamics*, Davis, CA.

Kabashnikov, V.P. and Kmit, G.I. (1979), *Appl. Spect.*, Vol. 31, pp. 963-967.

Kounalakis, M.E., Faeth, G.M. and Gore J.P. (1988), *Twenty-Second Symposium (International) on Combustion*. The Combustion Institute, Pittsburgh, PA, pp. 1281-1290.

Kounalakis, M.E., Sivathanu, Y.R. and Faeth, G.M. (1991), *ASME J. Heat Transfer*. Vol. 113, pp. 437-445.

Marion, M. and Temam, R., (1989), *SIAM J. Numer. Analysis*, Vol. 26, pp 1139-1157.

Mengüç, M.P. and Webb, B.W., (1993), in *Fundamentals of Coal Combustion*, Edited by L.D. Smoot, Chapter 5, Elsevier, Amsterdam, pp. 375-431.

Mengüç, M.P. and McDonough, J.M., (1994), "Regime Maps for Radiation-Turbulence Interactions", presented in the poster session, *Twenty-Fifth Symposium (International) on Combustion*, Irvine, CA, August 1994.

McDonough, J. M., Bywater, R. J. and Buell, J. C., (1984a), AIAA Paper 84-1674.

McDonough, J. M., Buell, J. C. and Bywater, R. J., (1984b), ASME Paper 84-WA/HT-16.

McDonough, J. M. and Bywater, R. J., (1986), *AIAA J.* Vol. 24, pp 1924-1930.

McDonough, J. M. and Bywater, R. J., (1989a). in *Forum on Turbulent Flows - 1989*, Bower and Morris (eds.), ASME FED-Vol.76, ASME, NY, pp. 7-12.

McDonough, J. M., Hylin, E. C., Catton, Ivan, Chan, Tony F. C. and Mathew, T., (1989), UCLA-ENG-6762N-87, School of Engineering and Applied Science, University of California, Los Angeles.

McDonough, J.M., Yang, Y. and Hylin, E.C. (1995), In *Proceedings of First Asian Computational Fluid Dynamics Conference*, Vol. 2, Hui et al.(eds.), Hong Kong University of Science and Technology, pp. 747-752.

McDonough, J. M. and Saito, K., (1995), to appear in *Int. J. Fire Sci. Tech.*

McDonough, J. M. and Wang, D., (1995), to appear in *Proceedings of Parallel CFD'94*, Kyoto, Elsevier Science, Amsterdam..

McMurtry, P.A. and Queiroz, M., (1993), in *Fundamentals of Coal Combustion*, L.D. Smoot, editor, Elsevier, Amsterdam, pp. 511-566.

Mitchell, A. R. and Griffiths, D. F., (1980), *The Finite Difference Method in Partial Differential Equations*, John Wiley and Sons, Chichester.

Moin, P. (1992), In *Studies in Turbulence*, Gatski et al.(eds.), Spring-Verlag, NY, pp. 223-228.

Ruelle, D. and Takens, F. (1971), in *Commun. Math. Phys.* Vol. 20, pp. 167-192

Tamanini, F., (1977), *Comb. Flame*, Vol. 30, pp. 85-101.

Viskanta, R. and Mengüç, M.P., (1987), *Progress in Energy and Combustion Science*, Vol. 13, pp. 97-160.

Yang, Y. and McDonough, J. M., (1992). in *Bifurcation Phenomena and Chaos in Thermal Convection*, Bau et al. (eds.), ASME HTD-Vol. 214, ASME, NY, pp. 85-92.