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A THREE-REGION, MOVING BOUNDARY MODEL OF A FURNACE FLAME

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DISCLAIMER

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ABSTRACT

This paper describes a new, efficient technique for computing first-order spatial dependence of a furnace flame. The technique, called the moving boundary flame model, creates dynamic state variables that track the size of the flame within the furnace. The approximation is appropriate for full plant training simulators, control system analysis, and engineering analyses in which a higher fidelity model than a point reactor model is needed. In comparison to the point reactor models, the one dimensional spatial dependence should improve the accuracy of distributed quantities such as heat transfer and reaction rates over the range fuel and air flow conditions that exist in normal and abnormal operation. The model is not intended to replace detailed multi-dimension flow models of the furnace. Although the flame model is a first principles model, the accuracy depends on data from a more detailed combustion simulation or experimental data for volume-averaged parameters such as the turbulent mixing coefficient for fuel and air, radiative and conductive heat transfer coefficients, and ignition and extinction conditions. These inputs can be viewed as tuning parameters used normalize the moving boundary model to a more accurate model at a particular operating point.

The result of the development is a successful flame model. A set of equations has been developed that are physically plausible as well as compact and easy to program. A numerical simulation using the system of equations produces a well-behaved solution. The eigenvalues for the solution are in the frequency range that is significant for controls and engineering analysis. At the same time, the system does not have any extremely fast states (large negative eigenvalues). This indicates that the model has the necessary dynamics for the problems of interest without any properties of a stiff system that would make numerical simulation difficult. Additional work is necessary to validate the model against experimental data or against a more accurate simulation of a furnace flame.

1. INTRODUCTION

The moving boundary flame model is a new, efficient technique for computing first-order, spatial dependence of a furnace flame. The model has dynamic state variables that track the position of the combustion zone within the furnace. The expected application for the model is dynamic system analysis for burner diagnostics and controls. Burner diagnostics and controls are expected to be areas for major development to reduce emissions and improve efficiency of commercial fossil power plants.

The power of the moving boundary formulation is in locating a point in space at which the process distinctly changes. Moving boundary models have been used for many years in modeling steam generators to locate the boundaries of the heat transfer regimes (subcooled, nucleate boiling, superheat).[1,2] The concepts for this model are drawn from that experience. The distinct boundaries for the combustion flame are 1) the point in space at which the fuel and air mixture is heated to the ignition temperature and 2) the point at which the fuel concentration reaches the extinction condition and combustion ends. By computing the position of these boundaries, the processes that depend on the spatial distribution can be represented more accurately.

The moving boundary model is determined by the choices of the flow rates at the boundary. The rest of the development simply solves the conservation equations over the control volumes for the state derivatives. A brief discussion of the conservation equations is provided to motivate the formulation without showing all the algebraic manipulations to get to the state derivative form. Reference 3 gives the entire derivation.

In addition to the conservation equations, we need the ideal gas law and empirical relationships for the combustion reaction rate and the heat transfer relationships to close the system of equations. In this report, functional relationships are given without derivation. The focus of this paper is on the feasibility and form of the moving boundary model not to present any particular fuel. The modeling features that depend on the fuel are the combustion rate modeling and the heat transfer modeling. Our choices are intended to represent coal combustion but essentially any fuel could be represented. The heat transfer and reaction rate models are sufficiently complex and accurate to show plausible dynamics and to show that the moving boundary formulation does not introduce any special limitations or restrictions for representing nonlinear, distributed processes within the flame.

2. MATHEMATICAL FORMULATION OF THE MODEL

Three concentric spherical regions, as shown in Fig. 1 are defined to approximate the geometry of the fireball in the furnace; pre-heat zone, combustion zone, and post-combustion zone. The pre-heat zone is defined as the volume in which the incoming air and fuel are heated to the ignition point. The combustion zone encloses the volume in which

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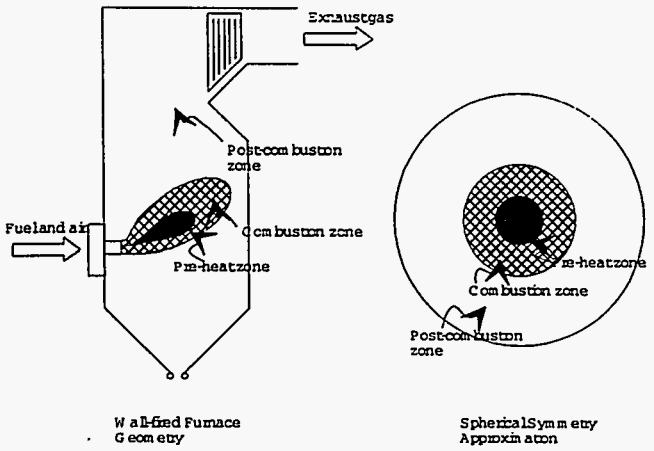
Figure 1. Flame Geometry Approximated by Spherical Symmetry



the chemical reaction takes place, and the post combustion zone is the remaining volume of the furnace.

The flows at the boundaries between regions are the quantities that define the material enclosed and hence define the dynamics of the moving boundaries. The control volume approach to conservation of mass and energy can then be used to produce a set of ordinary, initial-value, differential equations for the regions of the flame. For the three- region moving boundary model, the dynamic boundary flows are the flow leaving the preheat control volume and the flow leaving the combustion volume. The definition of the exit of the preheat region is that the temperature of the gas is at the ignition temperature. Hence, the flow at the boundary is equal to the rate that the fuel and air mixture in the region is heated to the ignition point. Written as an energy balance, the flow of fuel and air at the ignition temperature convects the same energy rate across the moving boundary out as heat is conducted and radiated into the region.

$$W_{PH}\, c_p\left(T_{ign} - T_{PH}\right) = \left(Q_{rad,PH} + Q_{cond,PH}\right) \tag{1}$$

where W_{ph} is the flow leaving the preheat region, c_p. is specific heat, $Q_{rad,PH}$ is the radiation component of energy transport, $Q_{rond,PH}$ is the conduction/diffusion component of energy transport, T_{ign} is the ignition temperature, and T_{PH} is the temperature of material stored in the preheat region.

In a similar fashion, the exit of the combustion region is the point in space at which the fuel/oxygen concentration is equal to the flame extinction point. The flow with respect to the boundary is proportional to the rate that the fuel and oxygen reach the extinction point. Hence, the flow leaving the combustion zone is proportional to the reaction rate. Since the reaction rate is formulated in mass of fuel consumed per unit time, the proportionality accounts for the fraction of oxygen and inert components carried with the fuel fraction. This flow can be written in the following form.

$$W_C = \frac{L}{F_{c,C}} \tag{2}$$

where L is the reaction rate in mass of carbon per second, $F_{c,C}$ is the mass fraction of carbon with respect to the total mass in the combustion region.

2.1 Conservation Equations

The conservation equations for energy and mass are used to derive a set of ordinary differential equations for the flame. One conservation of mass and one conservation of energy for each of three regions give six equations. Two volumes, three temperatures, and pressure give an equal number of state derivatives. The set of coupled ordinary differential equations form a linear system that can be solved for the unknown derivative terms. Conservation of species equations for the carbon and oxygen are used to compute the reactant concentrations needed for the carbon reaction calculation. Two species equations in the preheat and combustion regions add four state variables. This gives a total of ten state variables for the model of the flame.

The general control volume expressions for conservation of mass and energy for convection/ diffusion problems are routinely derived from the point equations by integrating over the control volume. The following are the standard forms for conservation of mass and energy using the upwind differencing approximation[4,5]. The only unusual characteristic of these equations in comparison to a fixed mesh spatial discretization is that the dynamic volume is included inside the derivative. Also, it is important to realize that the flow across a moving boundary must be interpreted as flow with respect to the moving boundary rather than flow with respect to a fixed frame of reference.

$$\frac{d\left(V\rho_{out}\right)}{dt} = W_{in} - W_{out} \tag{3}$$

$$\frac{d\left(V\rho_{out}c_pT_{out}\right)}{dt} = W_{in}c_pT_{in} - W_{out}c_pT_{out} - Q_{rad} - Q_{cond} + E + JV\frac{dP}{dt}. \tag{4}$$

where V is the volume (ft^3), T is temperature (°F), c_p. is specific heat (BTU/lbm-°F), ρ is density (lbm/ft^3), W is flow rate (lbm/sec), Q_{rad} is the sum of radiant heat transfer to other regions of the furnace (BTU/sec), Q_{cond} is conductive and diffusive heat transfer to other regions of the furnace (BTU/sec), P is pressure (psi), J is the heat equivalent of work, 778 BTU/lbf-ft, divided by 144 in^2/ft^2, E is the energy released by combustion (BTU/sec). The subscipts, *in* and *out*, indicate the entering and leaving boundaries of the control volume.

The energy storage term can be simplified by subtracting the mass equation multiplied by c_pT_{out} from the energy equation. Expanding the derivative on the left-hand side of (4) and performing the subtraction yields the form below. The advantage of this form of the energy equation is that it does not depend on the leaving flow, W_{out}, or the derivative of mass, $d(\rho V)/dt$. The unknown state derivative terms appear in linear terms on the left hand side of the equation.

$$V\dot{\rho}_{out}c_p\frac{dT_{out}}{dt} - JV\frac{dP}{dt} = W_{in}c_p\left(T_{in} - T_{out}\right) - Q_{rad} - Q_{cond} + E \tag{5}$$

The ideal gas law is used in the furnace to relate temperature, pressure, and density of the gas component of the fuel/gas mixture. To apply the ideal gas law, the mass of solid carbon must be subtracted from the total mass in the volume to obtain a mass equation for the gas alone. The assumption of perfect mixing and uniform velocity of fuel and gas allows the density and flow rate of the gas component to be defined in terms of the same mass fraction. Let the mass fraction of carbon (fuel) be represented by F_C. By definition, the mass fraction is the ratio of carbon mass to total mass.

$$F_c = \frac{M_c}{M_c + M_{gas}} = \frac{M_c}{M} \tag{6}$$

Converting the mass to the product of density and volume gives a similar relationship for the ratio of carbon density to mixture density. Also, since the velocities of the fuel and gas are assumed to be equal, the same mass fraction can be used to represent the ratio of carbon flow to total flow. Let v represent the flow velocity of the fuel air mixture, and A represent the area of a spherical shell.

$$F_c = \frac{\rho_c V}{\rho V} = \frac{\rho_c}{\rho} = \frac{\rho_c A v}{\rho A v} = \frac{W_c}{W} \tag{7}$$

Neglecting the volume occupied by fuel in comparison to the volume of gas, an equation for conservation of gas alone can be written as the following

$$\frac{d(V\rho_{gas,out})}{dt} = (1 - F_{c,in})W_{in} - (1 - F_{c,out})W_{out}. \tag{8}$$

The ideal gas law can be written in terms of density, temperature and pressure as the following.

$$\rho_{gas} = \frac{P}{fR(T+460)} \tag{9}$$

where f is a factor that converts mole density to mass density, R is the gas constant, $T+460$ is temperature in absolute units. Using the chain rule expansion of the storage term in (8) leads to a formula in terms of the state derivatives. As in the energy equation, the resulting form of the mass equation contains a linear combination of the unknown state derivatives on the left-hand side.

$$\rho_{gas,out}\frac{dV}{dt} + V\rho_{gas,out}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_{out}+460}\frac{dT_{out}}{dt}\right) = W_{in}(1 - F_{c,in}) - W_{out}(1 - F_{c,out}) \tag{10}$$

The system of equations for the mass and energy can be written out explicitly by adding the region subscripts to the general mass and energy equations. A few algebraic simplifications have also been made. The region subscripts are *EF* for entering furnace, *PH* for preheat region, *C* for combustion region, *PC* for post combustion, and *LF* for leaving furnace. When attached to a flow variable, the subscript indicates the flow leaving the region.

$$V_{PH}\rho_{PH}c_p\frac{dT_{PH}}{dt} - JV_{PH}\frac{dP}{dt} = W_{EF}c_p(T_{EF} - T_{PH}) \tag{11}$$

$$\rho_{gas,PH}\frac{dV_{PH}}{dt} + V_{PH}\rho_{gas,PH}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_{PH}}\frac{dT_{PH}}{dt}\right) = W_{EF}(1 - F_{c,EF}) - W_{PH}(1 - F_{c,PH}) \tag{12}$$

$$V_C\rho_C c_p\frac{dT_C}{dt} - JV_C\frac{dP}{dt} = W_{PH}c_p(T_{lgn} - T_C) - Q_{rad,C} - Q_{cond,C} + E \tag{13}$$

$$\rho_{gas,C}\frac{dV_C}{dt} + V_C\rho_{gas,C}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_C}\frac{dT_C}{dt}\right) = W_{PH}(1 - F_{c,PH}) - W_C(1 - F_{c,C}) \tag{14}$$

$$V_{PC}\rho_{PC}c_p\frac{dT_{PC}}{dt} - JV_{PC}\frac{dP}{dt} = W_C c_p(T_C - T_{GL}) - Q_{rad,PC} - Q_{cond,PC} \tag{15}$$

$$-\rho_{PC}\left(\frac{dV_{PH}}{dt} + \frac{dV_C}{dt}\right) + V_{PC}\rho_{PC}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_{PC}}\frac{dT_{PC}}{dt}\right) = W_C - W_{LF} \tag{16}$$

The set of six equations for mass and energy in the three regions are a linear system that can be expressed in matrix form.

$$AX = B \tag{17}$$

where $X = \left[\frac{dP}{dt}, \frac{dT_{PH}}{dt}, \frac{dV_{PH}}{dt}, \frac{dT_C}{dt}, \frac{dV_C}{dt}, \frac{dT_{PC}}{dt}\right]^T$

Because A is a relatively sparse matrix, the solution for X is readily obtained by Gaussian elimination.

2.2 Conservation of Carbon, Oxygen, and Inert Gas

The conservation of individual species in the control volume (e.g. carbon, oxygen, or inert) can be written in a balance form similar to the conservation of mass for the mixture. After applying the perfect mixing approximation, the fraction of carbon in the non-reacting preheat zone can be written as a first order lag.

$$\frac{dF_{c.out}}{dt} = \frac{W_{in}}{\rho V}\left(F_{c.in} - F_{c.out}\right) \qquad (18)$$

A similar derivation for oxygen gives the equivalent first order lag expression for the oxygen mass fraction. Note also that the mass fraction of the remaining inert components can be obtained by subtraction.

$$F_i = 1 - F_o - F_c$$

2.3 Quasi-steady Distribution Function of Carbon Concentration in Combustion Zone

The derivation of reaction rate in the control volume requires an approximate solution to the integral of the point equations for reaction rate over the control volume. With a control volume of the entire combustion region, we cannot know the transient distribution of the concentration. An excellent approximation of the transient shape is the shape function at steady state or quasi-steady function. The quasi-steady distribution function for reactant concentration is analogous in concept and method of derivation to the log-mean temperature difference formula for heat transfer in a counter-flow heat exchanger.[6,7] The quasi-steady shape function for reaction rate is an analytical solution of the steady state conservation of species equations for the carbon and oxygen and the total conservation of mass (assuming uniform velocity of fuel and gas). The resulting ordinary differential equation is separable and can be integrated analytically. The unburned carbon appears as a limit of integration in the integral over the carbon. In this model, we have assumed that unburned carbon is a constant and is quite small. The assumption is for convenience (and is not essential for solution of the moving boundary model). The objective is to determine the total, steady-state reaction rate of carbon in the combustion control volume from the point equations for reaction rate and conservation of reactant species. The local reaction rate of carbon is a function of the local concentration of carbon, oxygen and temperature.

$$l(z,T) = \tilde{n}_o(z)\tilde{n}_c(z)r(T), \qquad (20)$$

where $\tilde{n}_c(z)$ is the steady state mole density of carbon, $\tilde{n}_o(z)$ is the steady state mole density of oxygen, $r(T)$ is the temperature dependence of reaction rate, $l(z,T)$ is the reaction rate per unit volume, and z is the radial position.

The total reaction rate in the volume can be obtained from the above formula by integrating (32) for the local reaction rate over the combustion volume.

$$L = \int_{z_{PH}}^{z_C} l\left(T, n_o(z), n_c(z)\right) 4\pi z^2 dz, \qquad (21)$$

where L is the integral reaction rate over the combustion control volume.

The derivation for the reaction rate integral using the quasi-steady approximation is given in Reference 4. The result is the following.

$$L = \frac{rn_{ex}^2}{a}\frac{g\left(e^{aV} - 1\right)}{(g-1)\left(ge^{aV} - 1\right)}. \qquad (22)$$

where $g = \frac{\tilde{n}_{c.in} - n_{ex}}{\tilde{n}_{c.in}}$, $a = \frac{\rho r n_{ex}}{W}$,

2.4 Reaction Rate Temperature Function

The temperature dependence of the combustion rate, $r(T_R)$, includes the effects of both diffusion and chemical reaction processes on the reaction process. The oxygen diffuses through a depleted film surrounding the surface of the carbon particle and then reacts with the carbon. The overall reaction rate is commonly modeled using an electrical analogy of conductances in series to combine these effects.[8,9,10]

$$r(T_R) = \frac{3MW_c}{r_p \rho_c}\left(\frac{r_c r_d}{r_c + r_d}\right) \qquad (23)$$

where r_c is the chemical reaction component, and r_d is the diffusion component, and r_p is the radius of a coal particle. The diffusion and reaction conductances can be modeled by the following relations.

$$r_d = \left(\frac{D_0}{l}\right)\left(\frac{T_R}{T_0}\right)^m, \quad r_c = k_c\sqrt{T_R}\, e^{-\frac{B_c}{RT_R}},$$

r_d is the diffusion conductance, $m = 3/2$ for small particles moving slowly with respect to the gas (Stokes regime), l is the film thickness, and D_0 is the diffusion coefficient at T_0. r_c is the reaction conductance, k_c is a frequency constant, T_R is the temperature of reaction, B_c is the activation energy constant, and R is the ideal gas constant. The temperature of the reaction, T_R, is the local temperature of the carbon particle rather than the average mixture temperature in the control volume. As an approximation, the model uses the adiabatic flame temperature as the temperature of reaction.

2.5 Heat Transfer Equations

The heat transfer between regions and with the walls is due to both conduction and radiation processes. The formulas for heat transfer are computed using point (average) values of the temperature.

$$Q_{cond.i\text{-}j} = U_{i\text{-}j}A_{i\text{-}j}\left(T_i - T_j\right), \quad Q_{rad.i\text{-}j} = \sigma A_{i\text{-}j}\left(\varepsilon_i T_i^4 - \varepsilon_j T_j^4\right)$$

where U is the sum of diffusion and conduction heat transfer coefficients, A is the interface area between regions, σ is the Stephan-Boltzmann constant, and ε is the emissivity of the region. For the moving boundary regions, $A = 4\pi z^2$ where z radius of the spherical moving boundary region. i, j are subscripts indicating region. The subscripts take the values PH for preheat, C for combustion, PC for post-combustion, or W for wall. The subscript, i-j, means the boundary between the i-th and j-th regions.

3. RESULTS AND DISCUSSION

The flame model is programmed in the Advanced Continuous Simulation Language[11] (ACSL) to test its transient performance. The purpose of the transient tests is to show that the concept produces a workable model; that is to say that the model gives reasonable results and does not have undesirable numerical properties. No experimental data or

simulation data from another model are available to the author for comparison so no benchmarking could be done. Reasonable results from the model means that it conserves mass and energy and responds smoothly in the expected direction. Desirable numerical properties means that the model is only mildly nonlinear and that the integration (using the Gear Stiff integration algorithm) is accomplished with large time steps and few recalculations of the Jacobian.

To initialize the model, the power level, pressure, region volumes, and region temperatures were assigned arbitrary but reasonable values for a modern coal furnace. Then, the heat transfer coefficients and initial conditions were calculated to give steady state. The overall frequency coefficient of the combustion reaction was also normalized to achieve 99.9% combustion of the carbon in the volume assumed for the combustion zone. The normalization factor turned out to be very close to unity validating to some extent the assumed volumes. Steady state values from the model are given in Table 1.

Table 1. Steady state parameters for flame model

Parameter	Value	Units
Volume of preheat zone	2	ft^3
Volume of the combustion zone	100	ft^3
Volume of the furnace	1000	ft^3
Outlet pressure	14.2	psia
Furnace pressure	114.7	psia
Inlet temperature	482.2	°F
Preheat region temperature	482.0	°F
Combustion region temperature	3005.6	°F
Postcombustion region temperature	1928.5	°F
Heat of combustion	100,000,000	BTU/hr
Fuel flow	1.97	lbm/sec
Air flow	24.42	lbm/sec

To demonstrate the behavior of the flame model, transients were induced by step changes in the fuel/air flow rate, outlet pressure, and inlet temperature. Each parameter was stepped 10% from its steady state value while holding the remaining conditions constant. The dynamic response to each of these transients is given in a set of three plots showing temperatures, volumes, and pressure. The transients all show a well-behaved response. The increase in fuel/air flow is essentially a power increase. Figures. 2-4 show the expected increase in volume, temperature, and pressure. The step decrease in outlet pressure, Figs. 5-7, shows an increase in combustion volume due to decreased reactant density and associated decreases in temperature. Figures 8-10 show the response to an increase in inlet temperature. The preheat volume diminishes since less heat is required to reach the ignition point. The combustion volume and temperature increase by small amounts. The post-combustion temperature goes up an amount slightly less than the inlet temperature rise. Because of the increased temperature, heat transfer to the furnace walls is increased.

Figure 2. Step Change in Fuel/Air Flow: Preheat Region Temperature and Volume

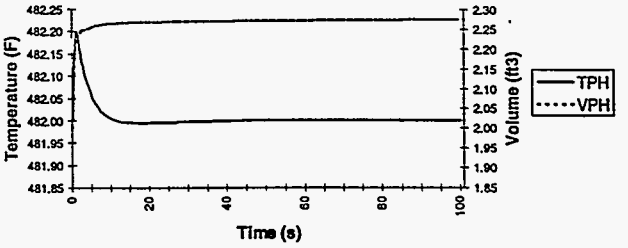


Figure 3. Step Change in Fuel/Air Flow: Combustion Region Temperature and Volume

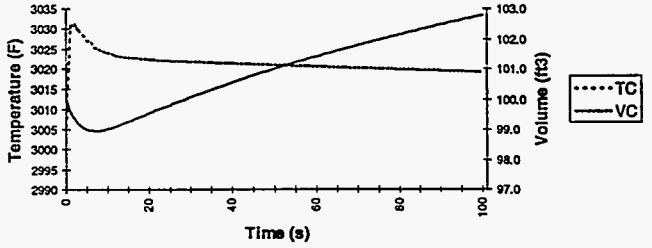


Figure 4. Step Change in Fuel/Air Flow: Post-Combustion Temperature and Furnace Pressure

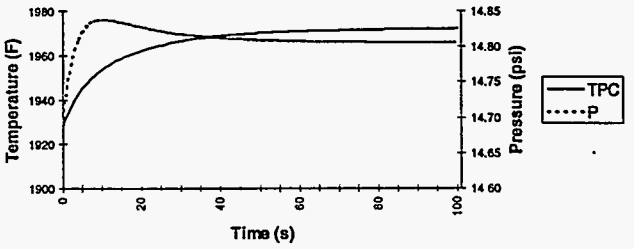


Figure 5. Step Change in Downstream Pressure: Preheat Region Temperature and Volume

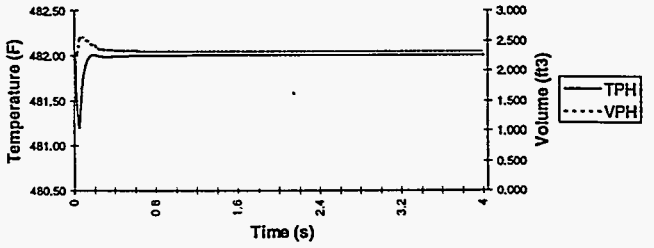


Figure 6. Step Change in Downstream Pressure: Combustion Region Temperature and Volume

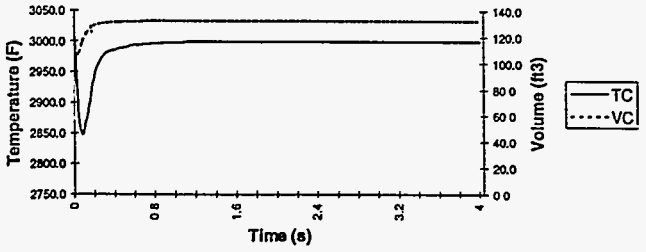


Figure 7. Step Change in Downstream Pressure: Post Combustion Temperature and Furnace Pressure

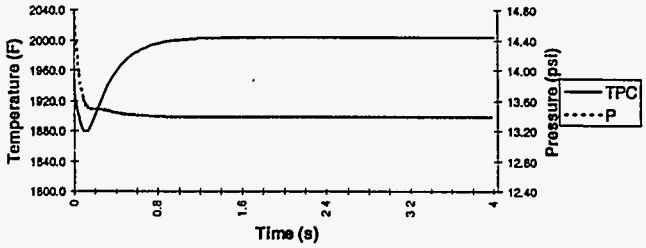


Figure 8. Step Change in Inlet Temperature: Preheat Region Temperature and Volume

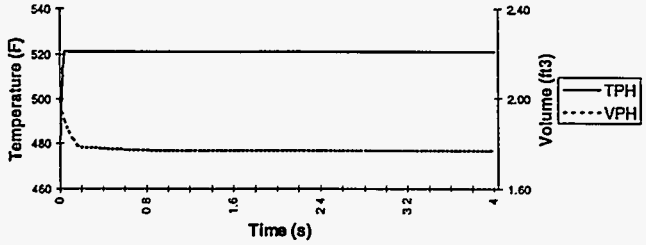


Figure 9. Step Change in Inlet Temperature: Combustion Region Temperature and Volume

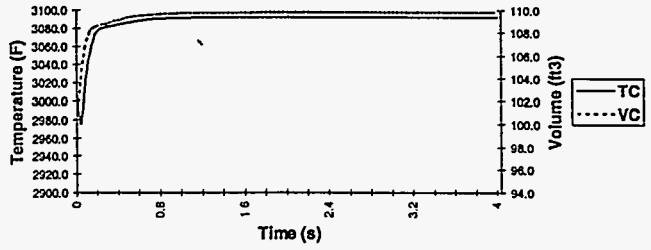
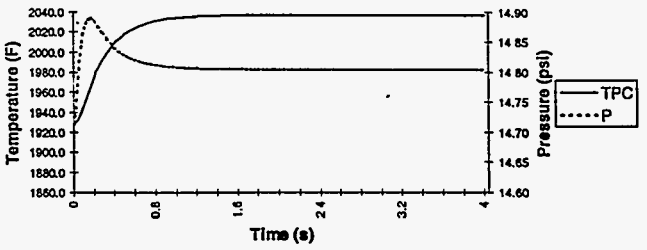


Figure 10. Step Change in Inlet Temperature: Post Combustion Temperature and Furnace Pressure



4. CONCLUSIONS

A three-region, moving boundary model of a wall-fired furnace flame has been presented. The model is shown to have robust numerical properties, easily simulating a variety of step change transients. The results are physically reasonable and numerical efficiency is excellent. These traits suggest that the moving boundary model can be very successfully incorporated into a full plant model of a fossil power plant. The anticipated improvements in comparison to point reactor models are more accurate transient dynamics of the plant.

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