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A Three-Region, Moving Boundary Model of a Furnace Flame

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

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DISCLAIMER

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CONTENTS

FIGURES

TABLES

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Executive Summary

This project developed a new, efficient technique for computing first-order, spatial dependence of a furnace flame. The technique, called the moving boundary flame model, creates a dynamic state variable that tracks the size of the flame within the furnace. Another innovative technique used in conjunction with the moving boundary technique is the quasi-steady spatial function. The quasi-steady spatial function provides an approximation of local concentrations of reactants which are then used for computing the combustion reaction rate. Although not developed in this demonstration, the spatial function also provides the necessary local conditions for computing other reaction rates such as NO_x production.

The approximations used in this model are appropriate for full plant training simulators, control system analysis, and engineering analyses requiring a full plant model. In comparison to 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 of 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 conditions. These inputs can be viewed as tuning parameters used to 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.

ABSTRACT

A dynamic model of a furnace flame is presented. The model simulates the preheat, combustion, and postcombustion regions of a wall-fired coal furnace. The set of nonlinear differential equations describing the flame dynamics are derived from the fundamental equations of conservation of mass and energy. The key approximations for flows across the moving boundary and spatial distribution functions for the carbon and oxygen concentrations in the combustion zone are developed. Sample results of transient calculations are presented.

1. INTRODUCTION

This paper develops a new, efficient technique for computing first-order, spatial dependence of a furnace flame. The technique, called the moving boundary flame model, creates a dynamic state variable that tracks the size of the flame within the furnace. Another innovative technique used in conjunction with the moving boundary technique is the quasi-steady spatial function. The quasi-steady spatial function provides an approximation of local concentrations of reactants which are then used for computing the combustion reaction rate. Although not developed in this demonstration, the spatial function also provides the necessary local conditions for computing other reaction rates such as NO_x production.

The approximations used in this model are appropriate for full plant training simulators, control system analysis, and engineering analyses requiring a full plant model. In comparison to 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 of 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 conditions. These inputs can be viewed as tuning parameters used to normalize the moving boundary model to a more accurate model at a particular operating point.

The flame model approximates the process of combustion in a wall-fired furnace for a power boiler. In a wall-fired furnace, the fuel and air enter through burner nozzles in the furnace wall. The mixture is heated to the ignition temperature, fuel and oxygen react to produce heat and combustion products, and the mixture of combustion gases exits the furnace into the gas path downstream of the furnace. The hot gases in the furnace conduct and radiate heat to the furnace walls.

The inputs or boundary conditions supplied by external modules or computations include flows entering and leaving, wall temperature, and fuel and air concentration at the inlet. The outputs are the furnace pressure, heat transfer rate to the walls, and the temperature and composition of gas leaving the furnace. Variables internal to the module compute the positions of the moving boundaries, the temperature, pressure, density, heat transfer rate, and other auxiliary relationships.

The feasibility of the moving boundary derivation hinges on defining the volume enclosed by the moving boundary and computing the distribution of properties, such as reactant concentration, within the volume. The control volume approach produces a set of ordinary, initial-value, differential equations. The key approximation in defining the volume for the moving boundary is selecting the flows with respect to the moving boundaries. These include the flow leaving the preheat control volume and the flow leaving the combustion volume. There are several methods for modeling these flows. The approach chosen in this model is the simplest. For the flow exiting the preheat zone, the flow is equal to the rate that the fuel and air mixture is heated to the ignition point. In a similar fashion, the flow leaving the combustion zone is equal to the rate that the fuel and air mixture burns. (Inert gases are carried off in proportion to their mass fraction in the fuel and air mixture.)

The second key approximation is the quasi-steady approximation for the spatial distribution of reactant concentration within the combustion zone. An approximate analytic solution of the steady state conservation equation for reactants is obtained. The solution gives the functional dependence of concentration on position. The concentration shape function is used in turn to compute an integral of the reaction rate within the

combustion zone. Although this paper presents only the reaction rate for the primary carbon-oxygen reaction, other distributed processes including heat transfer and other reactions such as the rate of reaction for pollution gases (e.g. NO_x) can be computed by the same technique.

2. MATHEMATICAL FORMULATION OF THE MODEL

The main advantage of the moving boundary formulation is in locating the 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).[1,2,3] The concepts for this model are drawn from that experience. The distinct boundaries for the combustion flame are 1) the point at which the fuel and air mixture is heated to the ignition point and 2) the point at which the reactants are consumed 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 approach interchanges the role of the concentration and position variables in the solution. In contrast to a conventional fixed mesh formulation that computes the time-varying concentration of carbon at a fixed point in space, the moving boundary formulation recasts the conservation of mass equation to compute the time-varying position of the combustion zone. The reaction rates, radiation, and conduction in turn depend on the appropriate flame radius, surface area, or volume variable.

To simplify the system of equations, only the solid carbon-oxygen reaction is considered in this model. The carbon reaction is the dominant energy release process and is slower than the reactions of volatile gases. Hence, the combustion of carbon encompasses a larger volume than the region over which volatile species react. Equations for all the other species, when they are added, will be built on the moving grid defined by the carbon moving boundary.

Three concentric spherical regions 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 the chemical reaction takes place, and the post-combustion zone is the remaining volume of the furnace.

2.1 PHENOMENA SIMULATED AND LIMITATIONS

The basic phenomena considered in the flame model and limitations that result are the following:

- The furnace flame is assumed to be a spherical shape (fireball) within the furnace walls as shown in Fig. 1. Spherical symmetry simplifies the flame to one-dimensional flow.
- The combustion of solid carbon particles is modeled. The combustion of volatile gases is neglected for simplicity in this demonstration model.
- A single average burner is modeled with the primary transport air being the only source of combustion air. Secondary and tertiary air sources are combined with primary air to simplify the geometry of the flame for this demonstration.
- Ignition conditions are approximated by a constant temperature. If the fuel-air mixture is heated to the ignition temperature within the furnace volume, then it is assumed to produce a stable flame.

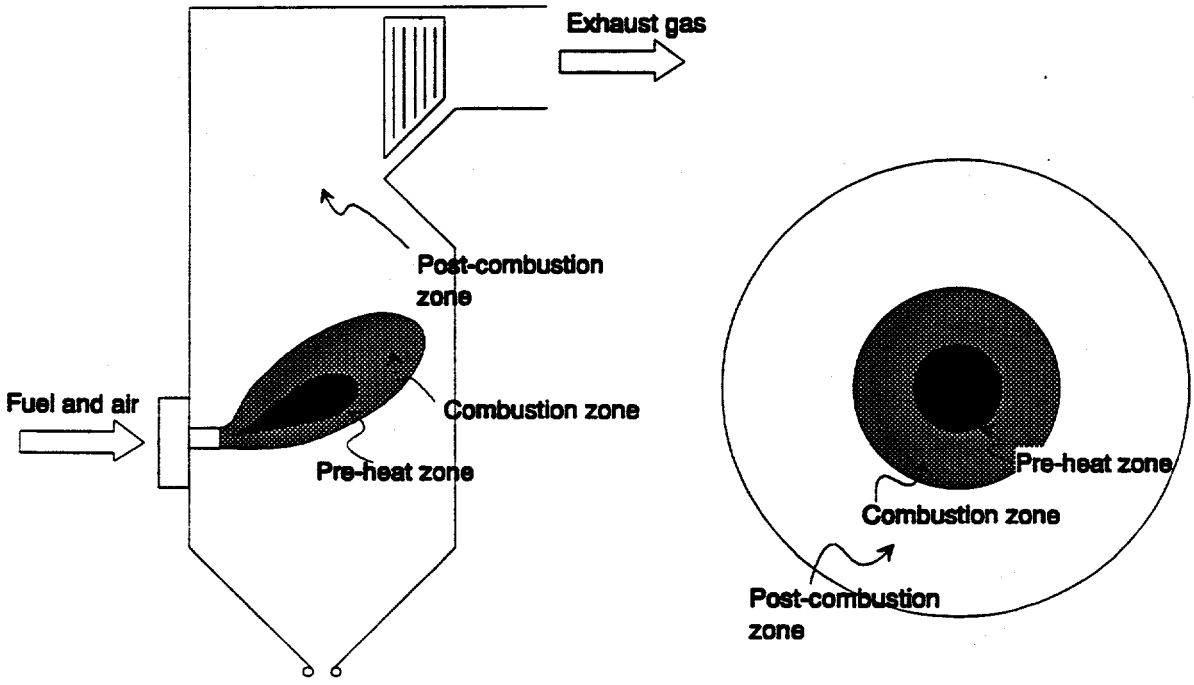

Fig. 1. Wall-fired furnace is approximated as a sphere.

- Reaction rate of carbon is based on the Parker and Hottel formula which includes conductances for oxygen diffusion and chemical reaction combined in series.

2.2 ASSUMPTIONS AND APPROXIMATIONS

- The quasi-steady shape functions for carbon concentration and temperature can be used as an approximation to the transient spatial dependence.
- The furnace gases behave as ideal gases and the mixture as an ideal gas mixture.
- Fuel and air entering the combustion zone are perfectly mixed.
- Carbon particles and transport air move at the same velocity.
- Gas flows do not reverse.
- All three regions exist at all times. (This means for example that the combustion zone does not increase beyond the furnace boundary making the post-combustion zone disappear.)
- The rate of combustion is limited by the primary carbon oxidation.
- The flow leaving the preheat region is equal to the rate that material in the preheat zone is heated to the ignition temperature.
- The flow leaving the combustion zone is equal to the rate the mixture burns. The exiting flow carries with it the mixture fraction of inert gas.
- The temperature of the carbon reaction can be approximated as the adiabatic flame temperature and treated as a constant over the combustion volume
- Pressure in the furnace is uniform.

2.3 MODEL DERIVATIONS

The following sections derive the conservation relations for the three regions of the furnace, the quasi-steady shape functions for carbon and oxygen concentration, and auxiliary relationships for reaction rate, heat transfer, and ideal gas law dependence of density, pressure, and temperature.

The conservation equations for energy and mass are used to derive a set of six ordinary differential equations for the flame (one conservation of mass and one conservation of energy for each of three regions). The six state derivatives that are defined by the mass and energy equations are two volumes, three temperatures, and pressure. 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 also defined. Conservation of carbon and oxygen in the preheat and combustion zones add a total of four state variables to the model. The concentration terms are used to compute the carbon reaction rate.

The conservation of momentum is eliminated from the model by assuming the pressure is uniform throughout the furnace. This approximation assumes the pressure and flow in the furnace reach equilibrium much faster than the processes of energy and mass transport. As discussed by Smoot[4], this approximation eliminates the possibility of simulating turbulence and flame stability. Turbulence and stability are important for burner nozzle design but are generally too fast for a control system to provide stable feedback. Consequently, the loss in high frequency fidelity is not severe for the problems of interest for this model.

2.3.1 General Conservation Equations for Mass and Energy

The general control volume expressions for conservation of mass and energy are routinely derived from the point equations by integrating over the control volume. The following forms assume no shaft work and neglect changes in kinetic and potential energy in the flame:

$$\frac{d(V\bar{\rho})}{dt} = W_{in} - W_{out} \tag{1}$$

$$\frac{d(V\bar{\rho}\bar{h})}{dt} = W_{in}h_{in} - W_{out}h_{out} - Q_{rad} - Q_{cond} + E + JV\frac{dP}{dt} \tag{2}$$

where V is the volume (ft^3)
h is the enthalpy (BTU/lbm)
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).

These equations must be manipulated into forms whose only unknowns are the state derivatives which we have chosen to be the temperatures, volumes and pressure in the flame. As discussed in Oran and Boris[5], the control volume equations are subject to numerical diffusion and the associated smearing of high frequency effects. For the purposes of this simulation, the goal is smoothness and stability. The control volume modeling is appropriate for the range of transients intended for the model.

The relationship of the average properties and outlet properties of a volume are approximated in this model by the perfect mixing approach. Perfect mixing of a control volume means that material entering the control volume mixes completely and instantly with the material already in the control volume. Therefore, the outlet properties of the volume (enthalpy, density, temperature, or reactant concentration) are equal to the average properties in the conservation equations.

$$\begin{aligned} h_{out} &= \bar{h} \\ \rho_{out} h_{out} &= \overline{\rho h} \\ T_{out} &= \bar{T} \end{aligned} \tag{3}$$

This is equivalent to upwind differencing or donor cell approximation. The resulting energy equation is the following,

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

Approximating the enthalpy of the mixture as a linear function of the temperature about (T_0, h_0)

$$h = c_p(T - T_0) + h_0 \tag{5}$$

leads to a conservation of energy equation in terms of the mixture temperature rather than enthalpy.

$$\frac{d(V\rho_{out}c_pT_{out})}{dt} = W_{in}c_pT_{in} - W_{out}c_pT_{out} - Q_{rad} - Q_{cond} + E + JV\frac{dP}{dt}. \tag{6}$$

The energy storage term can be simplified further by subtracting the mass equation multiplied by c_pT_{out} from the energy equation. Expanding the derivative on the left-hand side of (6) 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, $d(\rho V)/dt$.

$$V\rho_{out}c_p\frac{dT_{out}}{dt} - JV\frac{dP}{dt} = W_{in}c_p(T_{in} - T_{out}) - Q_{rad} - Q_{cond} + E \tag{7}$$

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.

$$F_c = \frac{M_c}{M_c + M_{gas}} = \frac{M_c}{M} \tag{8}$$

Converting the mass to the product of density and volume gives a similar relationship for the ratio of carbon density to mixture density.

$$F_c = \frac{\rho_c V}{\rho V} = \frac{\rho_c}{\rho} \tag{9}$$

Since the velocity 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.

$$F_c = \frac{\rho_c A v}{\rho_c A v + \rho_{gas} A v} = \frac{W_c}{W_c + W_{gas}} \tag{10}$$

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

$$\frac{d\left(V\rho_{gas,out}\right)}{dt} = \left(1 - F_{c,in}\right)W_{in} - \left(1 - F_{c,out}\right)W_{out} \tag{11}$$

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

$$\rho_{gas} = \frac{P}{fR(T+460)} \tag{12}$$

where f is a factor that converts mole density to mass density,
$f = (F_i/MW_i + F_o/MW_o)/F_c$
F is mass fraction,
MW is molecular weight,
i, o, and c are subscripts for inert gas, oxygen, and carbon respectively,
R is the gas constant
$T+460$ is temperature in absolute units

The partial derivatives of gas density with respect to pressure and temperature are:

$$\frac{\partial \rho_{gas}}{\partial P} = \frac{\rho_{gas}}{P}, \tag{13}$$

$$\frac{\partial \rho_{gas}}{\partial T} = -\frac{\rho_{gas}}{T+460} \tag{14}$$

Substituting the above equations into the conservation of gas mass gives the mass equation in terms of state derivatives.

$$\rho_{gas,out}\frac{dV}{dt} + V\rho_{gas,out}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_{out}+460}\frac{dT_{out}}{dt}\right) = W_{in}\left(1 - F_{c,in}\right) - W_{out}\left(1 - F_{c,out}\right) \tag{15}$$

2.3.2 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. The conservation of carbon can be written as:

$$\frac{d}{dt}\left(\rho_c V\right) = W_{c,in} - W_{c,out} \tag{16}$$

A more convenient form can be obtained by rewriting the density and flow rate in terms of the mass fraction of carbon multiplied by the total density and flow. The density and flow can be expressed in the following way,

$$\rho_c = F_c\rho, \quad W_{c,i} = F_{c,i}W_i$$

Substituting these terms in the conservation or carbon expression yields the following.

$$\frac{d}{dt}\left(\overline{F}_c\rho V\right) = F_{c,in}W_{in} - F_{c,out}W_{out} \tag{17}$$

We will use the perfect mixing approximation for the carbon concentration in the control volume.

$$F_{c,out} = \overline{F}_c \tag{18}$$

The perfect mixing approximation applied to the mass equation yields the following equation.

$$\frac{d}{dt}\left(F_{c,out}\rho V\right) = F_{c,in}W_{in} - F_{c,out}W_{out} \tag{19}$$

Multiplying the total mass equation (1) by the mass fraction, $F_{c,out}$, and subtracting from the above equation yields a simpler form.

$$\frac{dF_{c,out}}{dt} = \frac{W_{in}}{\rho V}\left(F_{c,in} - F_{c,out}\right) \tag{20}$$

In this form, the mass fraction for carbon is seen to be a first order lag. A similar derivation for oxygen gives the equivalent expression for the oxygen mass fraction

$$\frac{dF_{o,out}}{dt} = \frac{W_{in}}{\rho V}\left(F_{o,in} - F_{o,out}\right) \tag{21}$$

Note also that the mass fraction of the remaining inert components can be obtained by subtraction

$$F_i = 1 - F_o - F_c \tag{22}$$

2.3.3 Conservation Equations for Pre-Heat Region

The pre-heat zone is the volume at the center of the spherical flame immediately around the injection point. The mixture is heated to the ignition point in this region by radiation and conduction from the surrounding combustion region. The temperature of the mixture within the region is below the ignition point so no reaction or internal heat generation takes place in this region. The general equations for conservation of mass (7) and energy (15) are made specific to the preheat region by eliminating zero terms and adding the appropriate subscript designations.

Energy Equation

$$V_{PH}\rho_{PH}c_p\frac{dT_{PH}}{dt} - J\,V_{PH}\frac{dP}{dt} = W_{in}c_p\left(T_{in} - T_{PH}\right) \tag{23}$$

Mass Equation

$$\rho_{gas,PH}\frac{dV_{PH}}{dt} + V_{PH}\rho_{gas,PH}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_{PH}+460}\frac{dT_{PH}}{dt}\right) = W_{in}\left(1 - F_{c,in}\right) - W_{PH}\left(1 - F_{c,PH}\right) \qquad (24)$$

The flow leaving the region, W_{PH}, is defined as equal to the rate that material in the pre-heat zone is heated to the ignition temperature. The flow leaving can be written in equation form as the following:

$$W_{PH} = \frac{\left(Q_{rad,PH} + Q_{cond,PH}\right)}{c_p\left(T_{ign} - T_{PH}\right)} \qquad (25)$$

where $Q_{rad,PH}$ is the radiation component of energy transport
$Q_{cond,PH}$ 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

The energy equation is handled differently in the preheat region than in the other regions. The usual approach is for the average temperature to be equal to the outlet and the heat transfer terms to appear explicitly in the equation. The flow for W_{PH} in (25) is defined so that the convected energy, $Wc_p\Delta T$, is equal to the conducted/radiated energy, $Q_{rad}+Q_{cond}$. No energy is added to the material stored in the preheat zone. The energy is all added to mixture flowing out of the preheat region and into the combustion zone. It is as if there is a volumeless region between the preheat zone and combustion zone in which the all the energy transfer takes place. The energy equation (except for the PV term) is a first order lag that filters the temperature of the entering fuel air mixture with a time constant of $\rho V_{PH}/W$. This is a physically plausible treatment of the transport delay in the preheat region.

Carbon and Oxygen Equations

The general equations for the carbon and oxygen are derived in section 2.3.2. Including the subscripts for the preheat region makes the equation specific to the preheat zone.

$$\frac{dF_{c,PH}}{dt} = \frac{W_{in}}{\rho_{PH}V_{PH}}\left(F_{c,in} - F_{c,PH}\right) \qquad (26)$$

$$\frac{dF_{o,PH}}{dt} = \frac{W_{in}}{\rho_{PH}V_{PH}}\left(F_{o,in} - F_{o,PH}\right) \qquad (27)$$

2.3.4 Conservation Equations for the Combustion Region

The combustion zone is defined as the volume over which the oxygen and carbon react. The conservation of energy and mass equations for this regions can be expressed as the following:

Energy equation

$$V_C \rho_C c_p \frac{dT_C}{dt} - J V_C \frac{dP}{dt} = W_{PH} c_p (T_{ign} - T_C) - Q_{rad,C} - Q_{cond,C} + E \tag{28}$$

Mass equation

$$\rho_{gas,C} \frac{dV_C}{dt} + V_C \rho_{gas,C} \left(\frac{1}{P} \frac{dP}{dt} - \frac{1}{T_C} \frac{dT_C}{dt} \right) = W_{PH} (1 - F_{c,PH}) - W_C (1 - F_{c,C}) \tag{29}$$

The flow leaving the combustion region is defined as equal to the rate that combustion takes place.

$$W_C = \frac{MW_c L}{F_{c,C}} \tag{30}$$

where MW_c is the molecular weight of carbon
L is the reaction rate in moles per second
$F_{c,C}$ mass fraction of carbon in the combustion region

The factor of $F_{c,C}$ accounts for the inert gas and oxygen that are carried with the mixture out of the combustion zone.

Carbon and Oxygen Equations

The general equations for the carbon and oxygen are derived in section 2.3.2. Including the subscripts for the preheat region makes the equation specific to the preheat zone.

$$\frac{dF_{c,C}}{dt} = \frac{W_{PH}}{\rho_C V_C} (F_{c,PH} - F_{c,C}) \tag{31}$$

$$\frac{dF_{o,C}}{dt} = \frac{W_{PH}}{\rho_C V_C} (F_{o,PH} - F_{o,C}) \tag{32}$$

2.3.5 Conservation Equations for the Post-Combustion Region

The post-combustion zone is the volume of the furnace outside the fireball. The equations for this region are the following:

Energy equation

$$V_{PC}\rho_{PC}c_p\frac{dT_{PC}}{dt} - JV_{PC}\frac{dP}{dt} = W_C c_p\left(T_C - T_{GL}\right) - Q_{rad,PC} - Q_{cond,PC} \tag{33}$$

Mass equation

$$-\rho_{PC}\left(\frac{dV_{PH}}{dt} + \frac{dV_C}{dt}\right) + V_{PC}\rho_{PC}\left(\frac{1}{P}\frac{dP}{dt} - \frac{1}{T_{PC}}\frac{dT_{PC}}{dt}\right) = W_C - W_{PC} \tag{34}$$

The above equation does not segregate gas and solid components of the mixture as in the preheat and combustion zones. All the solid carbon is assumed to have reacted. The mass of reacted carbon is included in calculating the molecular weight of gas for the specific heat and density calculations.

Note also that the volume and derivative of volume of the post-combustion zone are related to the volume of the other regions.

$$V_{PC} = V_F - V_{PH} - V_C \tag{35}$$

and,

$$\frac{dV_{PC}}{dt} = -\left(\frac{dV_{PH}}{dt} + \frac{dV_C}{dt}\right). \tag{36}$$

2.3.6 Solution of the State Derivatives

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

$$AX = B, \tag{37}$$

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

The elements of A and B can be obtained from the equations above. Since A is a relatively sparse matrix, the solution is readily obtained by Gaussian elimination. The conservation of carbon and oxygen for the preheat and combustion zones add four state variables for a total of ten states in the carbon flame model.

2.4 QUASI-STEADY DISTRIBUTION FUNCTION OF CARBON CONCENTRATION

The derivation of the quasi-steady distribution function to approximate the local transient reactant concentration in the combustion zone is one of the important, innovative features of the model. The idea of the quasi-steady function is that a time dependent distribution in space can be approximated reasonably well by its shape at steady state. The quasi-steady distribution function is analogous in concept and method of derivation to the log-mean temperature difference formula for heat transfer in a counter-flow heat exchanger. The quasi-steady shape function works well with the moving boundary formulation because the distribution function depends explicitly on the position of the moving boundary.

2.4.1 Steady state equations for the carbon conservation

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 of the form.

$$l(z,T) = \eth_o(z)\eth_c(z)r(T), \tag{38}$$

- $\eth_c(z)$ Steady state mole density of carbon,
- $\eth_o(z)$ Steady state mole density of oxygen,
- $r(T)$ Temperature dependence of reaction rate,
- $l(z,T)$ Reaction rate per unit volume,
- z Radial position.

Assuming plug flow (no diffusion or turbulent mixing of constituents), the steady state conservation of carbon mass is the following:

$$\nabla\cdot\left(\eth_c \mathbf{v}\right) = -\eth_c\eth_o r. \tag{39}$$

- v Flow velocity of fuel and gas mixture,

Because we have simplified the combustion to a single oxidation reaction, mole concentration of oxygen is the following:

$$\nabla\cdot\left(\eth_o \mathbf{v}\right) = -\eth_c\eth_o r. \tag{40}$$

Since the derivatives are equal, the oxygen and carbon concentrations can only differ by a constant. Let n_{ex} be that constant representing the excess oxygen in the mixture. Therefore, the mole densities at any point are related by

$$\eth_o(z) = \eth_c(z) + n_{ex}. \tag{41}$$

Assuming spherically symmetric flow, the divergence of a vector function, f, is a scalar derivative with respect to the radial position, z, in the following form.

$$\nabla \cdot f = \frac{1}{z^2}\frac{d(z^2 f)}{dz}. \tag{42}$$

Incorporating these terms into (41) yields a one dimensional equation for the mole density of carbon.

$$\frac{1}{z^2}\frac{d(z^2 \hat{n}_c v)}{dz} = -\hat{n}_c(\hat{n}_c + n_\alpha)r. \tag{43}$$

Note that the overall conservation of mass at steady state is

$$\nabla \cdot (\rho v) = 0. \tag{44}$$

Approximating the density, ρ, as a constant, then the equation can be written as

$$\nabla \cdot v = 0, \tag{45}$$

or, in spherical coordinates

$$\frac{1}{z^2}\frac{d(z^2 v)}{dz} = 0. \tag{46}$$

The physical interpretation of (40) is that the flow through a spherical shell (or any closed surface) is a constant. The convenient way to express this result is in terms of the steady state flow:

$$4\pi\rho z^2 v = constant = W, \tag{47}$$

or

$$z^2 v = \frac{W}{4\pi\rho}. \tag{48}$$

Substituting this expression into the carbon concentration and noting that W is independent of z gives:

$$\frac{W}{4\pi\rho z^2}\frac{d\bar{n}_c}{dz} = -\bar{n}_c\left(\bar{n}_c + n_{ex}\right)r. \tag{49}$$

The term, r, is a rate conductance term that depends on temperature and pressure. The term is developed formally in Section 2.4.2. Because the temperature of the reaction is a complex function of position, the term presents a serious complication to the analytic integration of the above equation. The temperature depends on both local effects within the burning coal particle and global effects from the average temperature of the mixture. A rigorous treatment of the temperature dependencies of the reaction rate should couple the steady state temperature distribution function with the concentration function. However, an analytic solution of the problem with this degree of detail is not possible. A reasonable approximation is to assume the reaction takes place at the adiabatic flame temperature. The flame temperature, given by the following equation, assumes adiabatic combustion of the fuel and air. The combustion is assumed to consume all the available fuel or oxygen, whichever is limiting.

$$T_R = T_{ign} + \frac{H}{c_p W_{C,in}} Min\left[F_{C,c}W_{C,in}, \frac{F_{C,o}W_{C,in}}{\phi_{alf}}\right], \tag{50}$$

where T_R is the temperature of the reaction
T_{ign} is the ignition temperature,
H is the energy released per pound of carbon,
$F_{C,c}$ is the mass fraction of carbon entering the combustion zone,
$F_{C,o}$ is the mass fraction of oxygen entering the combustion zone, and
ϕ_{alf} is the stoichiometric air/fuel ratio.

Because combustion takes place within the carbon particle, the reaction is insulated from the surrounding media. Therefore, the adiabatic flame temperature is a reasonable approximation for the temperature dependence at the point of combustion.

Assuming a constant temperature over the volume for the conductance parameter allows reaction coefficient to be taken outside the integral. The equation for concentration can be separated into integrals depending the variables of integration.

$$\int_{\bar{n}_c(z_{in})}^{\bar{n}_c(z')} \frac{d\bar{n}_c}{\left(\bar{n}_c + n_{ex}\right)\bar{n}_c} = \frac{4\pi\rho r}{W_{PC,in}} \int_{z_{in}}^{z'} z^2 dz. \tag{51}$$

The quasi-steady shape function for carbon concentration is obtained by integrating both sides of the equation.

$$\bar{n}_c(z) = \frac{n_{ex}\bar{n}_{c,in}}{\left(\bar{n}_{c,in} + n_{ex}\right)e^{\frac{4\pi\rho r n_{ex}}{3W}\left(z^3 - z_{in}^3\right)} - \bar{n}_{c,in}}. \tag{52}$$

The above expression can be written in a simpler form by substituting

$$g = \frac{\bar{n}_{c,in} + n_{ex}}{\bar{n}_{c,in}}, \tag{53}$$

$$a = \frac{\rho r n_{ex}}{W}, \tag{54}$$

and

$$V = \frac{4\pi}{3}\left(z^3 - z_{in}^3\right). \tag{55}$$

The shape functions for carbon and oxygen concentration can be simplified to the following form with the above substitutions,

$$\bar{n}_c(V) = \frac{n_{ex}}{ge^{aV} - 1}, \tag{56}$$

and

$$\bar{n}_o(V) = \left(\frac{1}{ge^{aV} - 1} + 1\right) n_{ex}. \tag{57}$$

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

$$L = n_{ex}^2 \int_0^{V_c} \frac{1}{\left(ge^{aV} - 1\right)}\left[\frac{1}{\left(ge^{aV} - 1\right)} + 1\right] dV, \tag{58}$$

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

Integrating the expression for L gives the following formula for total reaction rate in the combustion volume.

$$L = \frac{r n_{\alpha}^2}{a} \frac{g\left(e^{aV} - 1\right)}{(g-1)\left(g e^{aV} - 1\right)}. \tag{59}$$

2.4.2 Reaction Rate Function

The combustion rate of carbon particles is limited by the processes of diffusion and chemical reaction. The oxygen diffuses through the film surrounding the surface of the carbon particle and then reacts with the carbon. The rate coefficients can be combined as conductances in series. The diffusion conductance can be modeled by the following relation.

$$r_d = \left(\frac{D_0}{l}\right)\left(\frac{T_R + 460}{T_0}\right)^m \tag{60}$$

where $m = 3/2$ 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.

The reaction coefficient using the Parker-Hottel formulation is the following[6]:

$$r_c = k_c \sqrt{\left(T_R + 460\right)}\, e^{-\frac{B_c}{R\left(T_R + 460\right)}}, \tag{61}$$

where 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 conductances in series can be combined algebraically as the following

$$r_{CO} = \frac{r_c r_d}{r_c + r_d} \tag{62}$$

The reaction coefficients are formulated as a rate per unit surface area, such that

$$\textit{Reaction rate per unit surface area} = r_{CO} n_o \tag{63}$$

For our control volume model, the surface reaction rate must be converted to a reaction rate per unit volume. Let s_{α} be the surface area per unit volume, then

$$l = s_{ex} r_{CO} n_o \tag{64}$$

The surface area per unit volume can be derived in the following way.

$$\begin{aligned} s_{ex} &= \textit{Surface area of one particle} \cdot \textit{No. of particles per unit volume} \\ &= 4\pi r_p^2 \cdot \frac{\textit{Mass of carbon per unit volume}}{\textit{Mass of one particle}} \\ &= 4\pi r_p^2 \cdot \frac{\rho_{C,c}}{\frac{4}{3}\pi r_p^3 \rho_c} \\ s_{ex} &= \frac{3\rho_{C,c}}{r_p \rho_c} \end{aligned} \tag{65}$$

where r_p is the average carbon particle radius,
$\rho_{C,c}$ is the average density of carbon in the combustion control volume, and
$\rho_{c,solid}$ is the density of solid carbon.

Note that the mole density, n_c, is related to the density of carbon in the control volume by the relationship,

$$\rho_{C,c} = MW_c n_c \tag{66}$$

where MW_c is the molecular weight of carbon. Thus the equation for surface area per unit volume becomes

$$s_{ex} = \frac{3MW_c n_c}{r_p \rho_c} \tag{67}$$

Collecting the modeling terms from (56) and (61) in the reaction rate equation (58) yields the following formula for l

$$l = \frac{3MW_c}{r_p \rho_c} \left(\frac{r_c r_d}{r_c + r_d} \right) n_c n_o. \tag{68}$$

By comparison to the form needed in (32) , the temperature dependence factor, r, is found to be

$$r = \frac{3MW_c}{r_p \rho_c}\left(\frac{r_c r_d}{r_c + r_d}\right) \tag{69}$$

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 rather that the quasi-steady distributed values. The quasi-steady methodology can be applied to the heat transfer process (and in fact was attempted); however, the integrals are not solvable analytically. Methods of numerical solutions were not investigated due to lack of time. Instead, the solutions using average values for temperature are selected.

Conduction for heat transfer between gas regions is intended to represent both conduction and diffusion processes of heat transfer since both depend on the first power of temperature difference. The heat transfer coefficient represents the sum of the conduction and diffusion coefficients.

$$Q_{c,ij} = U_{ij} A_{ij} \left(T_i - T_j\right) \tag{70}$$

where U is the sum of diffusion and conduction heat transfer coefficients
A is the interface area between regions. For the moving boundary regions, $A = 4\pi z^2$ and z is the 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, $i6j$, means the boundary between the i-th and j-th regions.

The radiation terms are defined using similar nomenclature.

$$Q_{r,ij} = \sigma A_{ij} \left(\varepsilon_i T_i^4 - \varepsilon_j T_j^4\right) \tag{71}$$

where σ is the Stephan-Boltzmann constant,
ε is the emissivity of the region.

3. RESULTS AND DISCUSSION

The flame model is programmed in the Advanced Continuous Simulation Language[7] (ACSL) to test its transient performance. The purpose of the transient tests is to determine 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 bench marking could be done. Reasonability means that model responds smoothly in the expected direction. Desirable numerical properties mean that the

model is only mildly nonlinear and that the integration is accomplished with large time steps and few recalculations of the Jacobian.

The equations presented in this paper are coded into the ACSL language. The integration of the system of differential equation is then performed using any one of several provided by ACSL. The results shown here were integrated using the Gear Stiff algorithm, but other integration methods can also be used.

To initialize the model to steady state, the conduction/diffusion coefficients are calculated to give zero temperature and volume derivatives in the preheat, combustion, and post-combustion zone. The fixed (estimated) quantities in the initialization calculation are the power level, volumes, and temperatures of the system. The overall frequency coefficient of the combustion reaction was also normalized to achieve complete combustion 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 the 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	14.7	psia
Inlet temperature	482.2	EF
Preheat region temperature	482.0	EF
Combustion region temperature	3005.6	EF
Postcombustion region temperature	1928.5	EF
Heat of combustion	100,000,000	BTU/hr
Fuel flow	1.97	lbm/sec
Air flow	24.42	lbm/sec

In the model, all the boundary conditions (inlet flow, concentration, and temperature; and wall temperature) except outlet flow are held constant. To allow outlet flow to equilibrate naturally to changes in furnace pressure, an orifice flow equation is used to compute the outlet flow rate. The downstream pressure is treated as a constant. The orifice flow equation is the following:

$$W_{PC} = k_{out}\sqrt{\rho_{PC}(P - P_{OUT})} \tag{72}$$

where P is the furnace pressure computed by the flame model.
P_{OUT} is a constant
ρ_{PC} is the outlet density computed by the flame model
k_{out} is the orifice flow loss coefficient

The orifice coefficient is chosen to give outlet flow equal to the inlet flow.
The flame model has good numerical properties for simulation. It is not particularly nonlinear. Except for one complex pair, the flame model's eigenvalues are negative and real. This usually indicates a system that is easy to integrate numerically. Also, the eigenvalues are in the frequency range of interest for control system dynamics indicating the features that are included are appropriate for control system analysis. Eigenvalues of the system linearized about the steady state point are given in Table 2.

Table 2: Eigenvalues for the Moving Boundary Flame Model Linearized at Conditions in Table 1.

	Real	Imaginary
1	-3.6043	
2	-21.309	
3	-21.309	
4	-17.054	+/-13.033
6	-30.239	
7	-221.80	
8	-289.214	
9	-289.214	
10	-289.321	

To demonstrate the behavior for a wide range of perturbations, transients induced by step changes in the fuel/air flow rate, outlet pressure, and inlet temperature are investigated. Each parameter is 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. Figs. 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. Figs 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

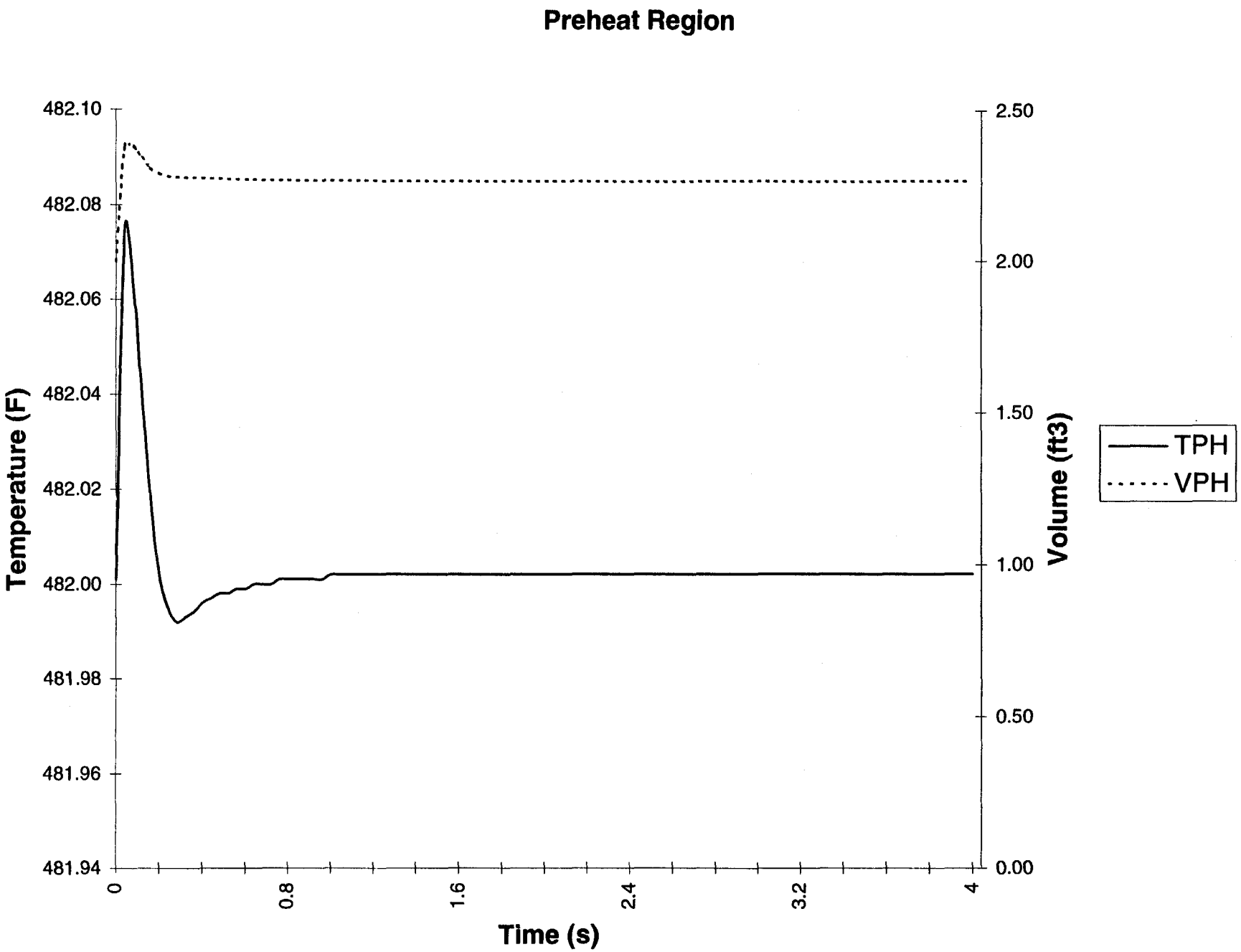

Fig. 2. Temperature and volume of the preheat region following 10% increase in fuel/air flow .

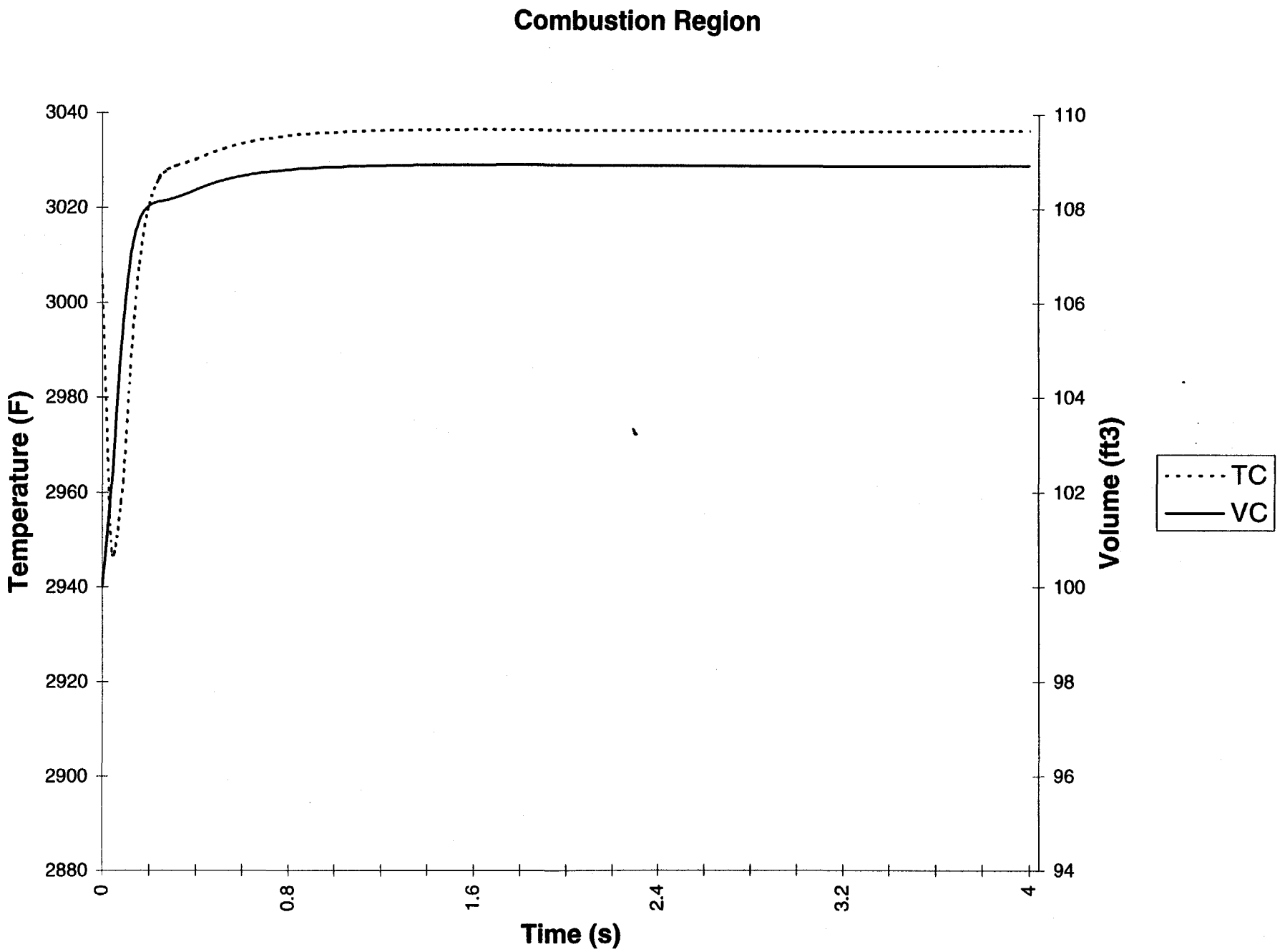

Fig. 3. Temperature and volume of the combustion region following 10% increase in fuel/air flow.

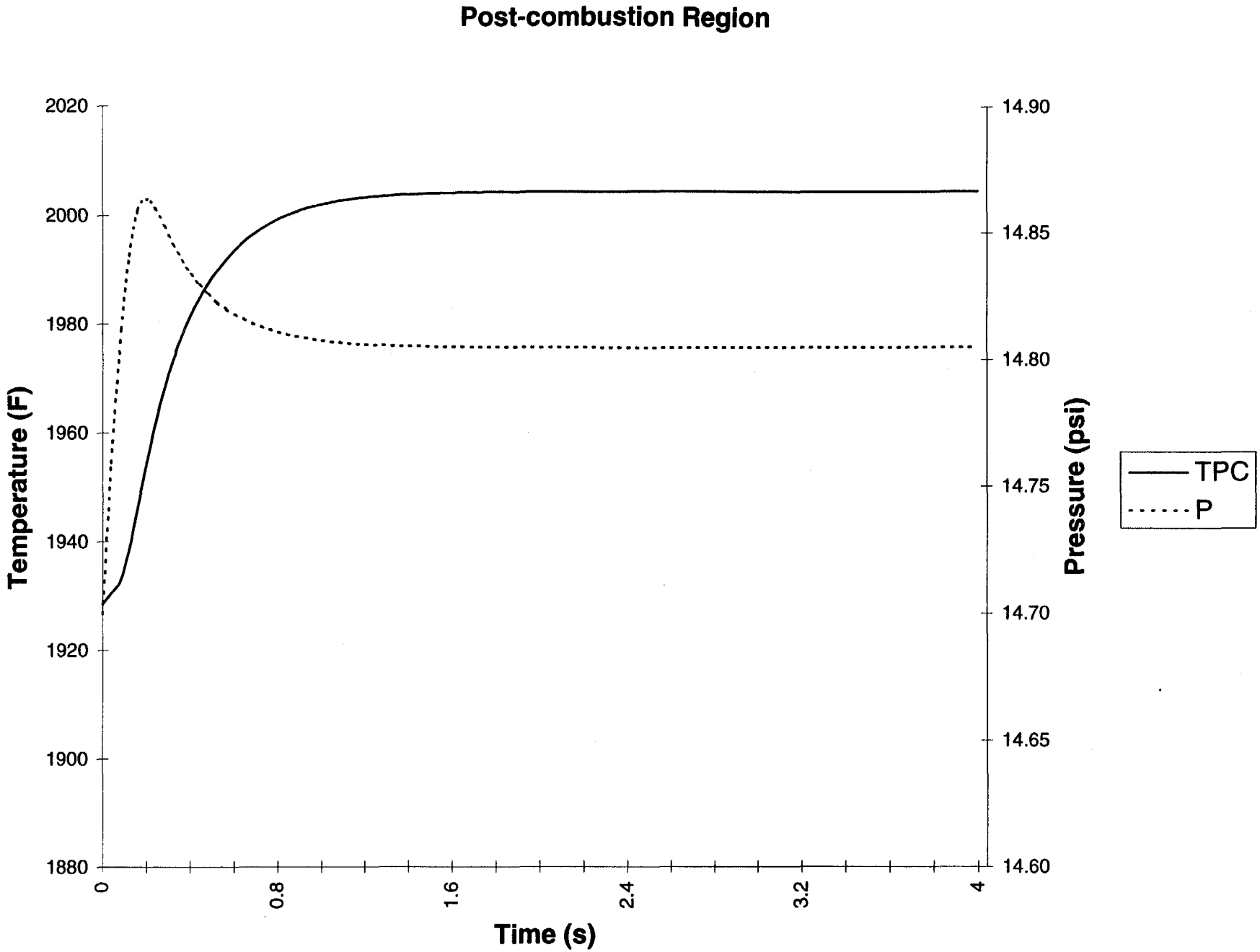

Fig. 4. Temperature and pressure in the post-combustion region following a 10% increase in fuel/air flow.

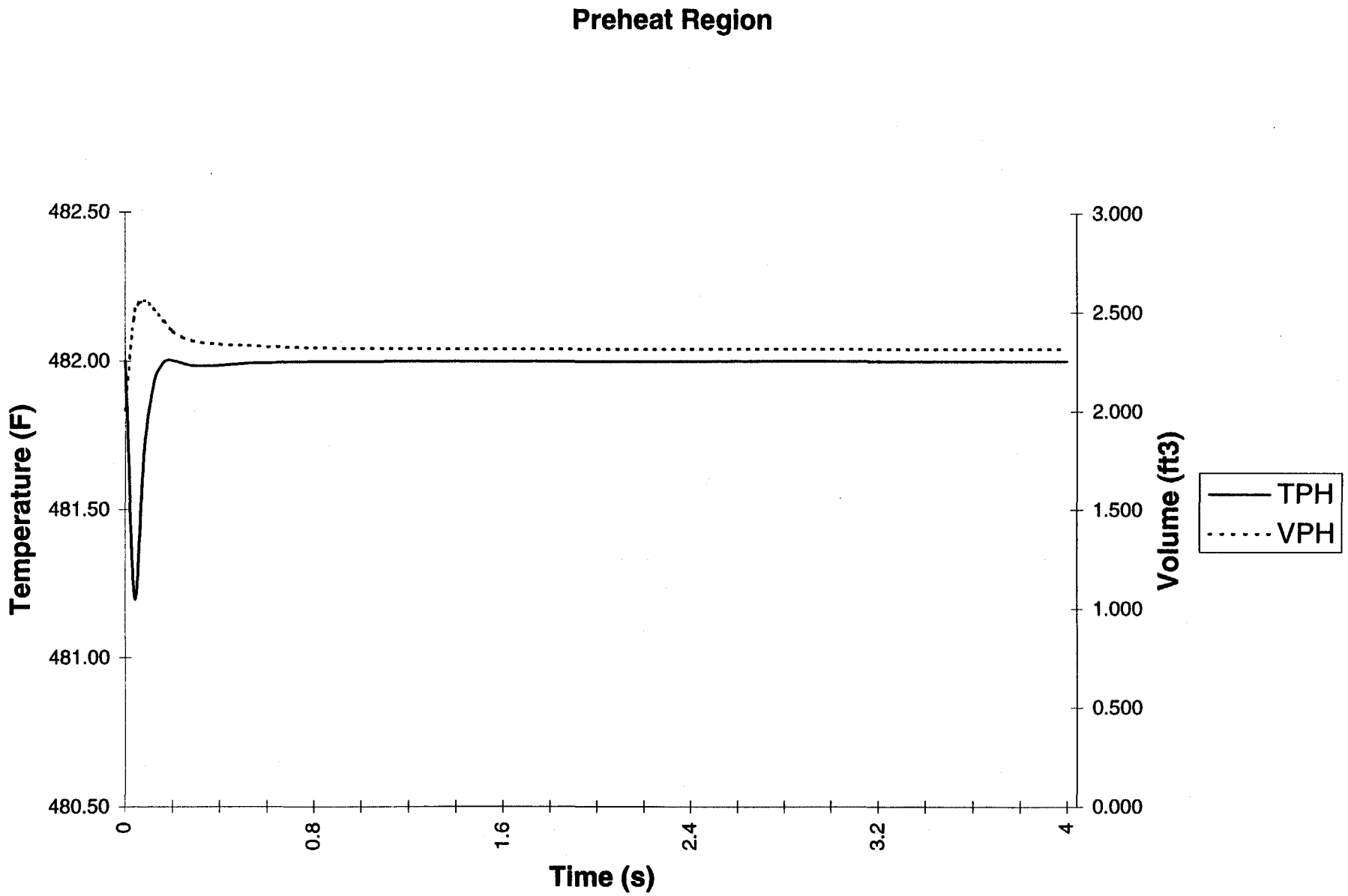

Fig. 5. Temperature and volume of the preheat region following a 10% decrease in back pressure .

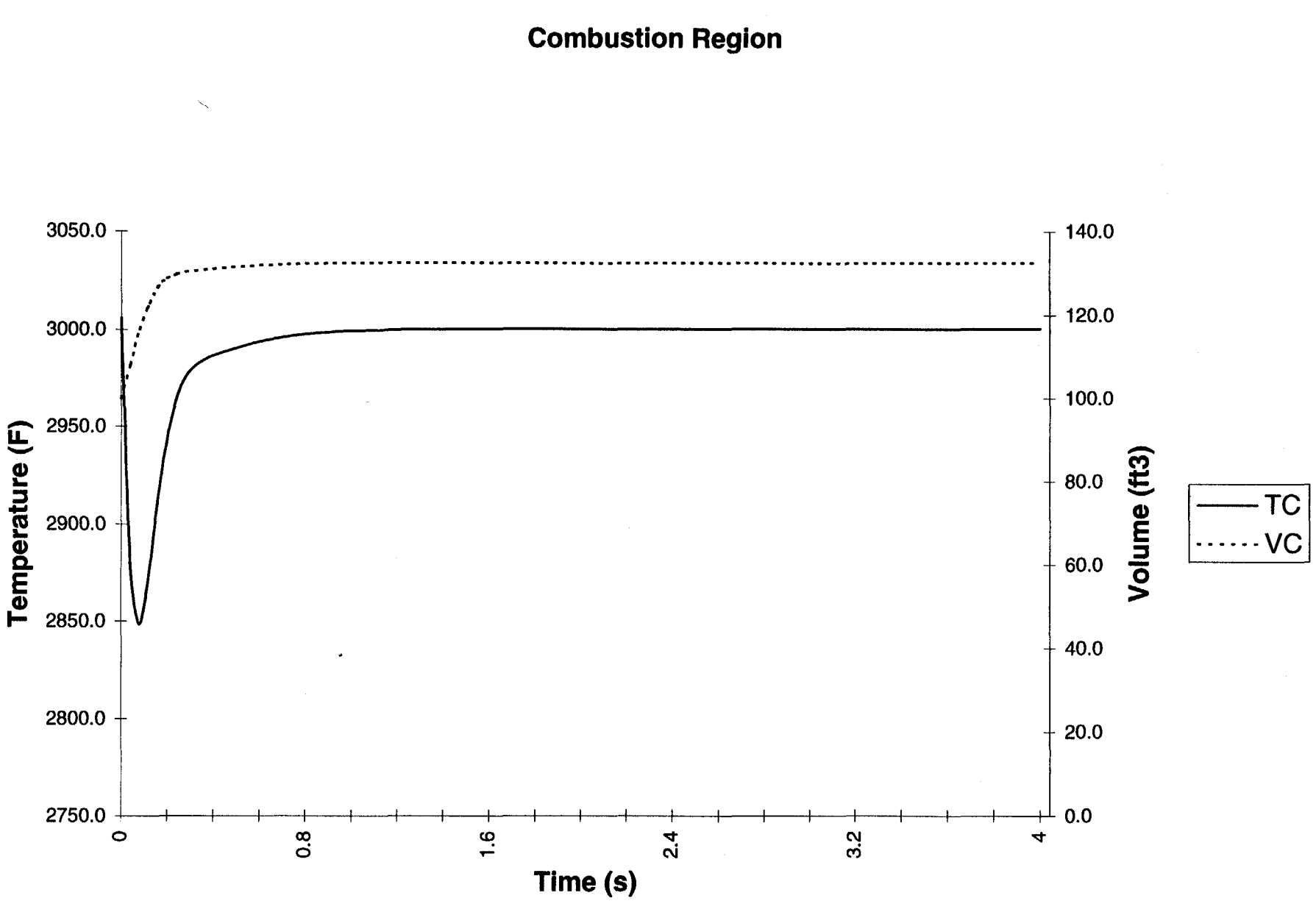

Fig. 6. Temperature and volume of the combustion region following a 10% decrease in back pressure .

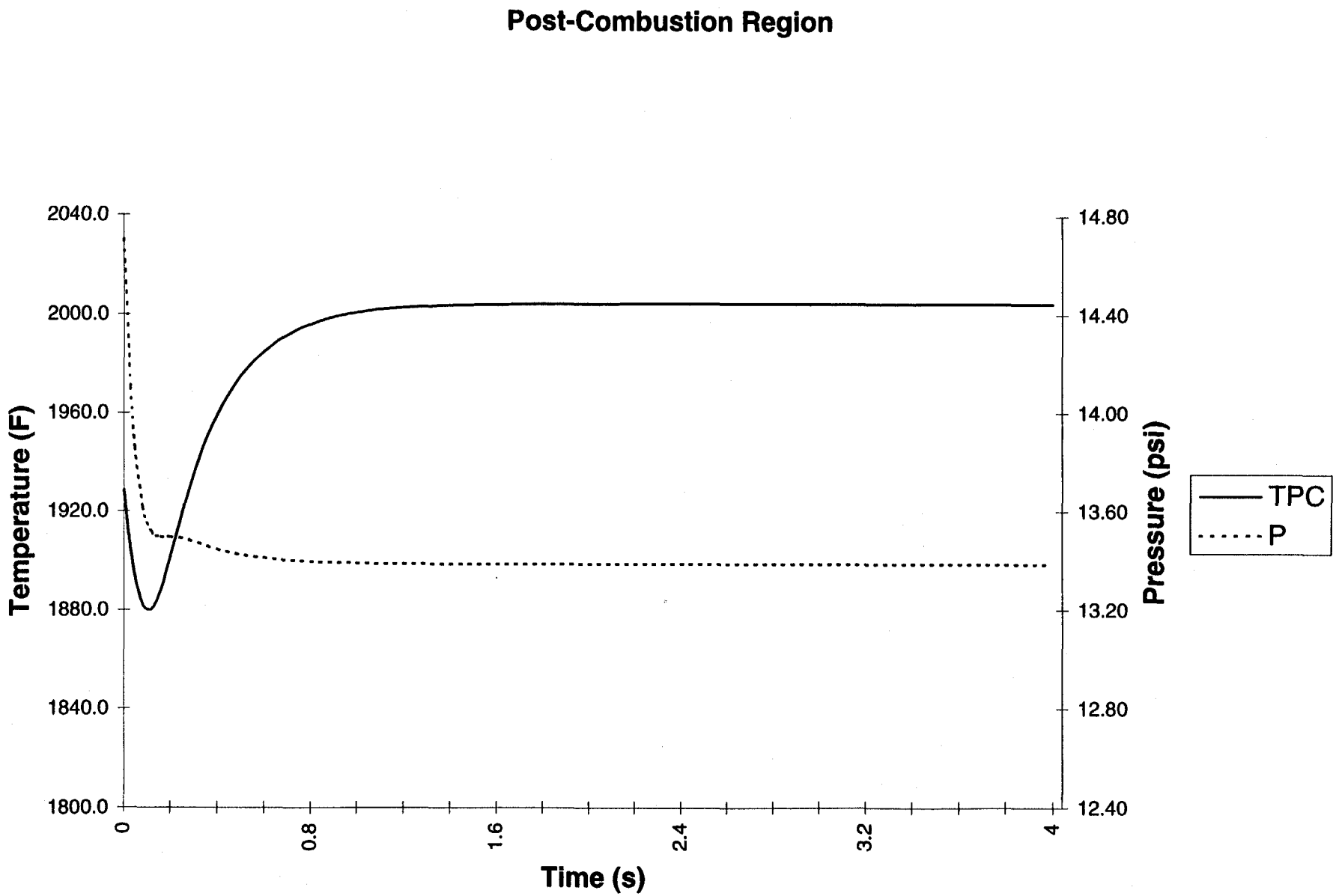

Fig. 7. Temperature and pressure in the post-combustion region following a 10% decrease in back pressure .

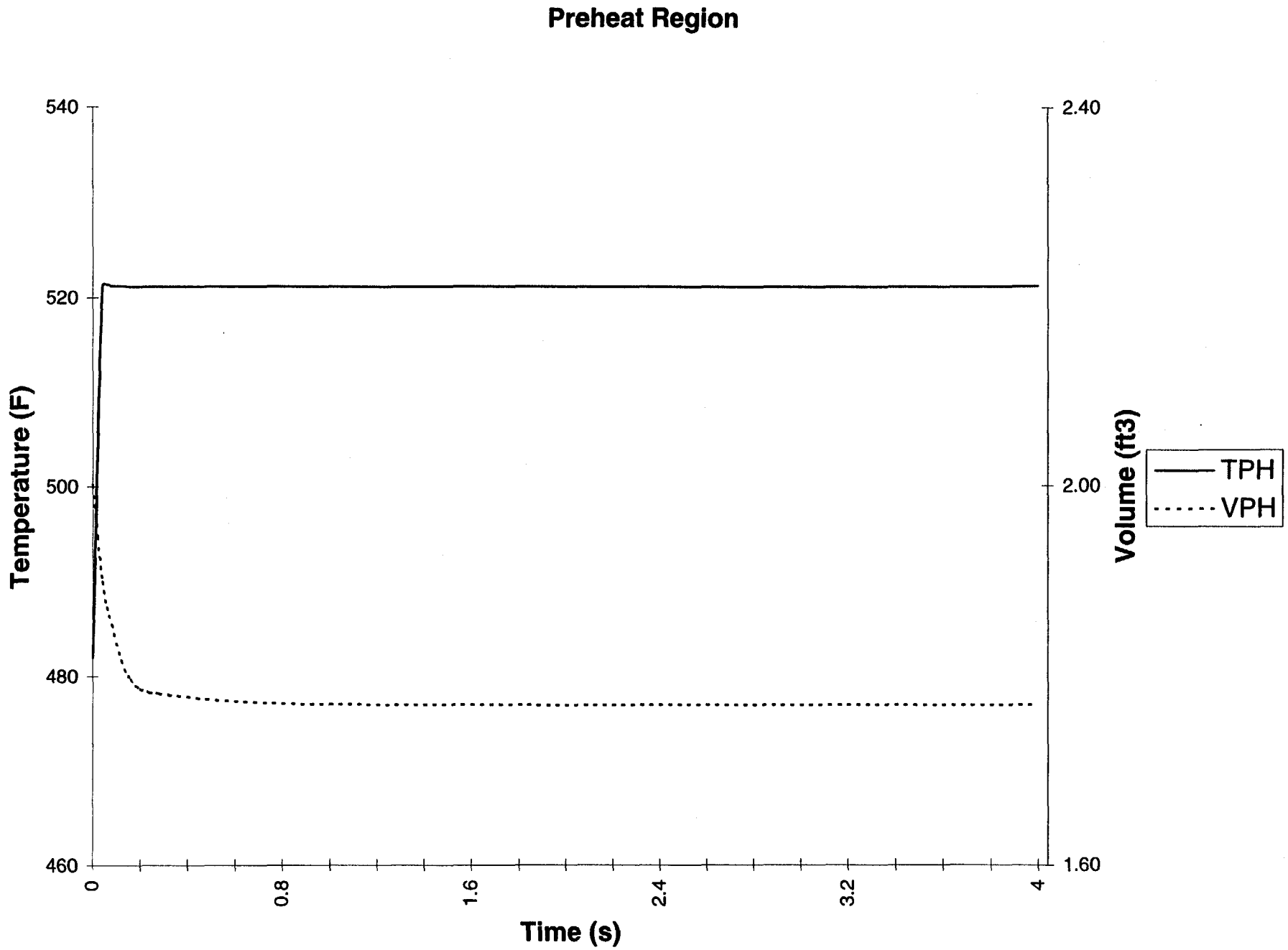

Fig. 8. Temperature and volume of the preheat region following a 10% increase in fuel/air temperature.

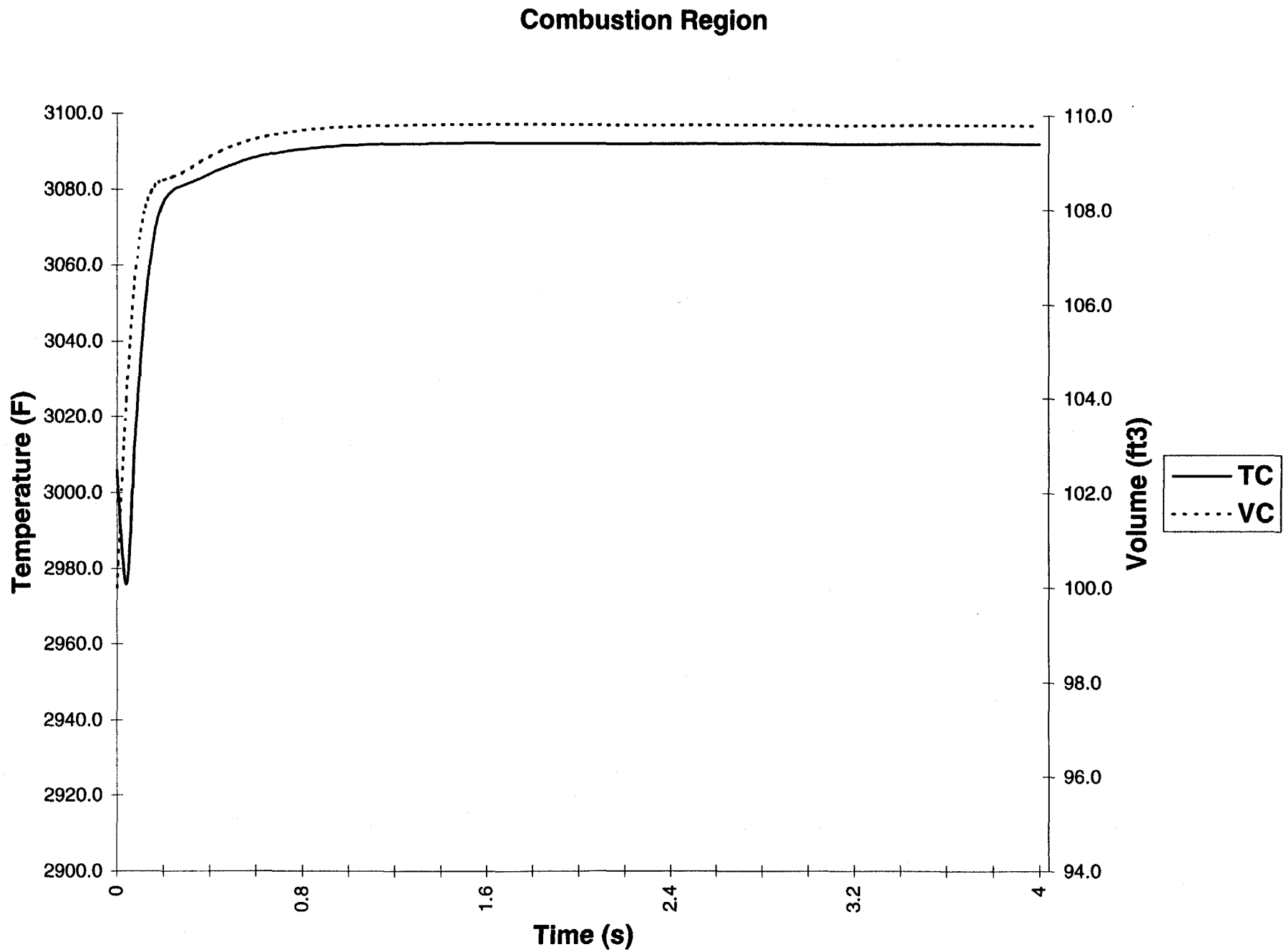

Fig. 9. Temperature and volume of the combustion region following a 10% increase in fuel/air temperature .

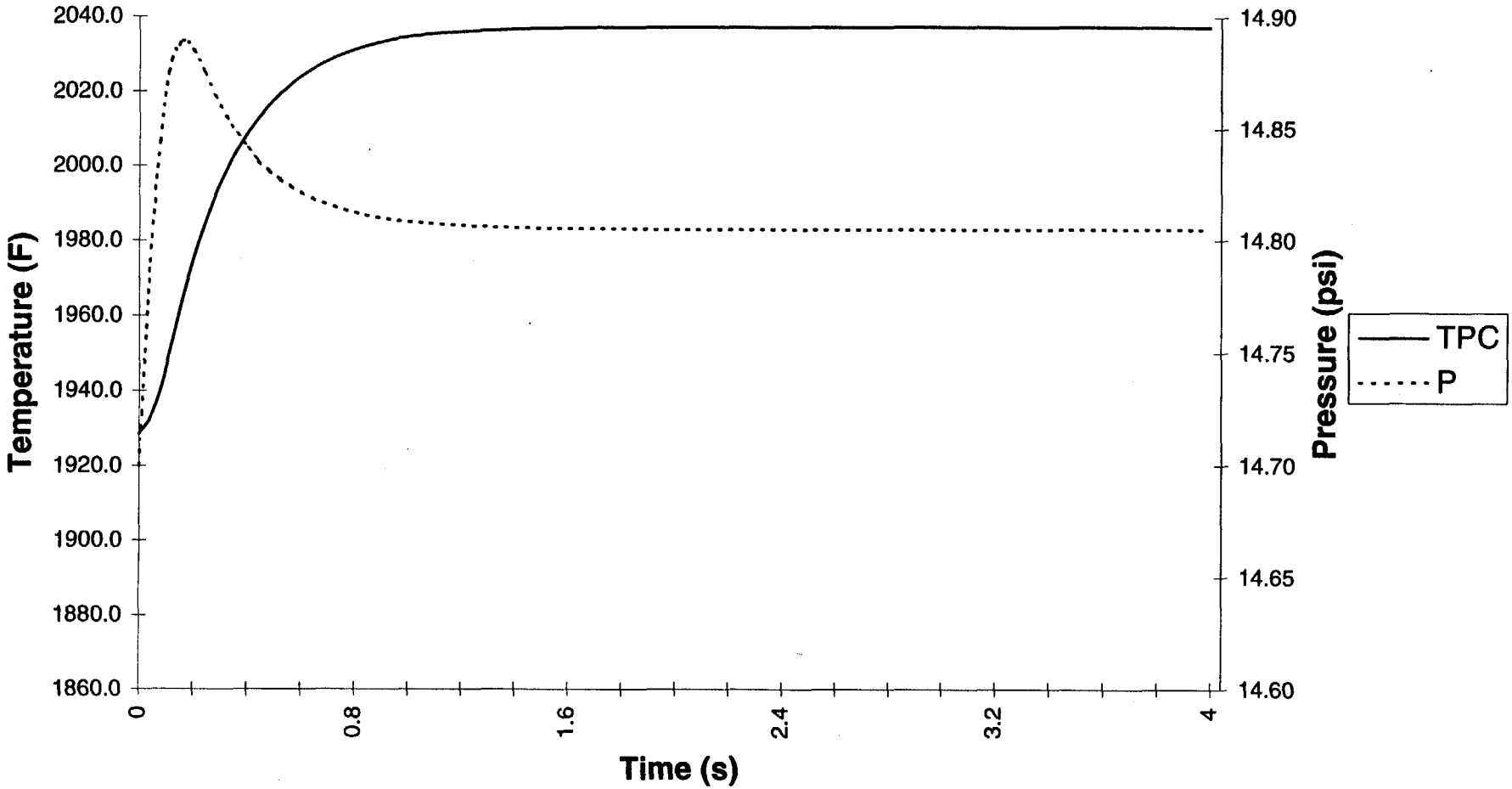

Fig. 10. Temperature and pressure of the post-combustion region following a 10% increase in fuel/air temperature .

increase 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.

The dynamic response of most variables is characterized by fully damped response or an overshoot and approach to equilibrium. These are all hyperbolic system responses. One interestingly different response is the volume of the combustion zone. Typically, this variable moves first in the opposite direction of its final equilibrium. This is a non-minimum phase response. With a non-minimum phase system, it is difficult to achieve stability and fast (high-gain) control at the same time. Moreover, a point-reactor model would not be capable of simulating this behavior. The dynamic response of the moving boundary flame model is needed to analyze and design the control system correctly.

4. CONCLUSIONS

A three-region, moving boundary model of a wall-fired furnace flame has been presented. The conservation equations for the moving boundary control volumes and quasi-steady concentration functions are derived. The resulting modeling equations are compact and relatively simple to program in a simulation language such as ACSL.

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 and the added capability to model spatially dependent processes such as formation of thermal NO_x.

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