

## A MODEL FOR PREDICTING THE GENERATION RATE AND DISTRIBUTION OF PRODUCTS OF COMBUSTION IN TWO-LAYER FIRE ENVIRONMENTS

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### ABSTRACT

A model is developed for predicting the generation rates of oxygen, fuel, and other products of combustion in rooms containing fires. The model is called the Generalized Global Equivalence Ratio Model (GGERM). It extends the steady state global equivalence ratio model established previously from steady-state data of several experimental studies. After describing the GGERM in detail, a concise algorithm is outlined for implementing it in two-layer zone-type compartment fire models. With the algorithm in place, such models could be used to simulate the distribution of combustion products in single or multi-room fire environments. In an example application, the GGERM is used to simulate the time-dependent environment, including that of steady-state, in some of the above-mentioned experimental studies. For arbitrary experimental conditions and under the assumption of complete stoichiometric combustion, solutions for concentrations of products of combustion are obtained and presented. The solutions are used to predict the time-to-extinguishment of a burning methane fuel source embedded in an initially ambient-atmosphere upper layer.

### NOMENCLATURE

$c_{FUEL,U}^{(MAX)}$  maximum possible  $c_{FUEL,U}$ , taken as 1

$c_{k,L} [c_{k,U}]$  mass fraction of product k in the lower [upper] layer

$c_{k,REACTOUT}$  mass fraction of product k in the reactor outflow

$c_{k,REACTOUT,STOICH}$   $c_{k,REACTOUT}$  for complete stoichiometric combustion

$c_{k,REACTOUT}^{(SS)} [c_{k,U}^{(SS)}]$   $c_{k,REACTOUT} [c_{k,U}]$  for steady state

$c_{k,REACTOUT}^{(SS,FIT)}(\phi)$  correlation functions fitted to experimental mass fraction data

$c_{OXY,U}^{(MAX)}$  maximum possible  $c_{OXY,U}$ , taken as 0.232

$f_k(\phi)$  Eq. (9)

$f_k^{(STOICH)}$   $f_k(\phi)$  for stoichiometric combustion

$m_L [m_U]$  total mass in lower [upper] layer

$\dot{m}_{FEEDBK}$  mass flow rate to the reactor from the accumulator

$\dot{m}_{FEEDBK,I}$   $\dot{m}_{FEEDBK}$  for conditions of Case I, I = 1, 2, or 3

$\dot{m}_{FEEDBK}^{(1)} [\dot{m}_{FEEDBK}^{(3)}]$  characteristic  $\dot{m}_{FEEDBK,1} [\dot{m}_{FEEDBK,3}]$

$\dot{m}_{FLOWIN} [\dot{m}_{FLOWOUT}]$  total mass flow rate into [out of] the upper layer

$(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}$  stoichiometric fuel-to-oxygen ratio

$\dot{P}_{k,FEEDBK}$  mass flow rate of product k into the reactor from the accumulator

$\dot{P}_{k,FLOWIN} [\dot{P}_{k,FLOWOUT}]$  sum of flow rates of all components of product k into [out of] layer

$P_{k,L} [P_{k,U}]$  mass of product k in the lower [upper] layer

$\dot{P}_{k,L} [\dot{P}_{k,U}]$  net rates of product k to the lower [upper] layer

$\dot{P}_{k,REACTIN}$  net mass flow rate of product k into the reactor

$\dot{P}_{k,REACTOUT}$  net mass flow rate of product k out of the reactor

R ideal gas constant for air

r  $(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}$

$T_{AMB} [T_U]$  temperature of ambient [upper layer]

t time

$t^*$	characteristic value of $t$ , Eq. (74)
$t_{EXT}$	$t$ at extinction of $CU_4$ flame
$V$	volume of the collector
$\alpha_{FUEL}, \alpha_{OXY}$	coefficients in $m_{FEEDBK}$ equation
$\beta$	dimensionless parameter
$\mu$	dimensionless value of $m_U$
$\rho_U$	density of the upper layer
$\sigma$	transformed value of $\tau$
$\tau$	dimensionless value of $t$
$\phi$	global equivalence ratio, Eq. (7)
$\phi^{(SS)}$	steady state $\phi$ , Eq. (19)
$\phi_{FUEL}, \phi_{OXY}$	Eqs. (26), (27)
$\sigma_{EXT}$	$\sigma$ at extinction of $CH_4$ flame
$\psi_k, \psi_{FUEL}, \psi_{OXY}$	dimensionless $c_{k,U}, c_{FUEL,U}, c_{OXY,U}$
$\dot{\omega}_k$	mass generation rate of product $k$

## INTRODUCTION

This paper presents a general model usable in two-layer zone-type compartment fire analyses, for predicting the generation rate and accumulation of combustion products throughout a multi-room facility. The model is called the Generalized Global Equivalence Ratio Model (GGERM).

### The Extended Upper-Layer in a Room Containing a Fire

Consider a multi-room compartment fire and assume an upper-layer/lower-layer zone-type description of the environment in each of the rooms. As indicated in Figure 1, for the purpose of describing the combustion

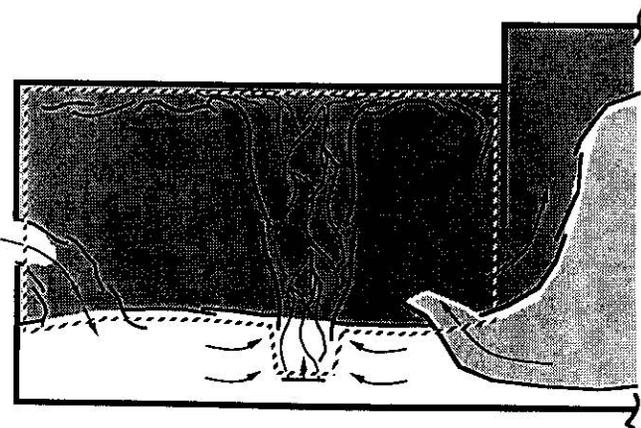


Fig. 1. The extended upper layer in a room of fire origin which includes the assumed negligible-volume fire plume.

process, the fire and plume, which may protrude into the lower layer, is taken as part of the upper-layer zone. Also, the volume of any such protrusion is assumed to be negligible compared to the total volume of the room. Thus, as defined by Quintiere (1989), all combustion processes in any room with a fire take place in the

upper layer. The actual combustion process in this extended upper-layer zone will be modeled here as in a well-stirred reactor (Spalding, 1979) with relatively rapid flow-through and corresponding negligible residence time.

### An Overview of the GGERM

Presented here is a brief overview of the essential features of the GGERM, the details of which are presented at length in the remainder of the paper.

The goal of the GGERM is to estimate net rates of change of mass of combustion products  $k$  in the upper layer,  $dP_{k,U}/dt$ , for any room containing a fire in an arbitrary multi-room fire scenario. As depicted in Figure 2, the model has two components: the accumulator,

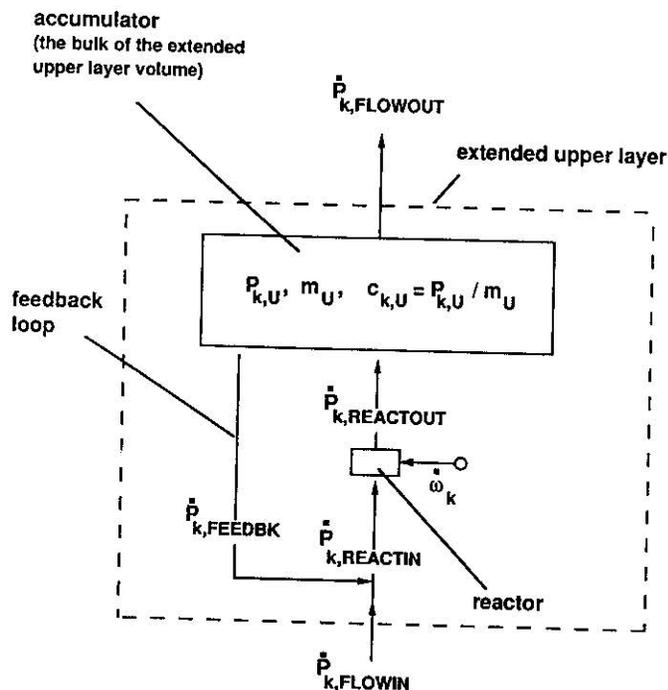


Fig. 2. The model of combustion and flow dynamics in the extended upper-layer of Figure 1.

which simulates the generally unsteady average upper layer environment, and the quasi-steady reactor, depicted in Figure 3, which simulates the actual combustion processes taking place there.

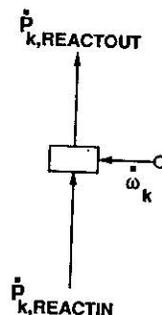


Fig. 3. An isolated view of the reactor of Figure 2.

The material flowing into and out of the extended upper layer generally includes various amounts of the combustion products  $k$  associated with a fuel of interest and other inert flow components. The actual inflow and outflow of product  $k$ ,  $\dot{P}_{k, \text{FLOWIN}}$  and  $\dot{P}_{k, \text{FLOWOUT}}$ , respectively, would be determined from compartment fire modeling considerations which are beyond the scope of this paper. These rates are assumed to be known.

As indicated in Figure 2, all of the flow into the layer is modeled as immediately "entering" the reactor where it participates in the reaction process. Also participating in the reaction is some of the bulk upper layer atmosphere. This is depicted in Figure 2 by the "feedback loop" flow which is also seen to "enter" the reactor. A critical feature of the overall model is the means of evaluating the feedback mass flow rate,  $\dot{m}_{\text{FEEDBK}}$ . This is presented in Eqs. (36)-(47).

The global equivalence ratio,  $\phi$ , is introduced as a normalized ratio of the rates of fuel to oxygen entering the reactor.  $\phi$  is defined and determined according to Eq. (7). Then the rate of generation of an arbitrary product  $k$ ,  $\dot{\omega}_k$ , is found from Eq. (9), where the  $f_k$  functions for the fuel would be determined from steady state experiments of the type carried out by Beyler (1986a, 1986b), Toner, Zukoski, and Kubota (1986), and Zukoski et al (1989, 1991). Having obtained the  $\dot{\omega}_k$ , conservation of species leads to the desired result for  $dP_{k,U}/dt$ . This is obtained from Eqs. (1) and (4).

#### THE VARIABLES COMPUTED IN A COMPARTMENT FIRE MODEL

At an instant of time of interest let  $P_{k,U}$  and  $P_{k,L}$  be the amount of product of combustion  $k$  in the upper and lower layers, respectively, of a room containing a fire.

Together with hydrostatic pressure at some datum elevation in the room, the elevation of the layer interface, and the total mass in the layers, it is convenient to use the  $P_{k,U}$ 's and  $P_{k,L}$ 's as basic variables in two-layer zone-type fire models [see, e.g., Cooper and Forney (1990)]. Also included in the basic solution variables are the pressures, interface elevations, masses, and  $P_{k,U}$ 's and  $P_{k,L}$ 's of all other rooms of the facility. While a  $P_{k,U}$  and  $P_{k,L}$  would correspond typically to the mass of product  $k$ , as is the case here, it could also correspond to some other extensive property, e.g., total number of particles of product  $k$ .

Variables derived from the basic variables are also required in analyses of the fire environment. For example, the density of the layer can be calculated from the layer interface elevation (i.e., layer volume) and layer mass. Similarly, the mass concentration of a product  $k$  in the upper layer,  $c_{k,U}$ , would be calculated from the values of  $P_{k,U}$  and upper-layer mass,  $m_0$ .

In a compartment fire model, generic equations for conservation of product  $k$  in the upper and lower layers are (Cooper and Forney, 1990):

$$dP_{k,U}/dt = \dot{P}_{k,U} \quad (1)$$

$$dP_{k,L}/dt = \dot{P}_{k,L} \quad (2)$$

where  $\dot{P}_{k,U}$  and  $\dot{P}_{k,L}$  represent the net rates of product of combustion  $k$  flowing to the upper and lower layer, respectively. These terms represent the sum of transfers of product  $k$  to the respective layers from all plumes, jets, near-boundary flows, combustion zones, and other isolated or distributed sources considered and taken into account in any particular zone fire model.

It is noteworthy that the number of types of flow and heat- and mass-transfer phenomena taken into account, and the detail and sophistication with which such phenomena are modeled are key distinguishing features between one zone fire model and another.

Since generation of products due to combustion processes are assumed to occur only in the extended upper layer,  $\dot{P}_{k,U}$ , but not  $\dot{P}_{k,L}$  can include generation-rate contributions due to combustion.

This paper presents a general model for including combustion processes in Eq. (1). It is applicable for general use in two-layer zone-type analyses of compartment fire scenarios. The model incorporates and extends to arbitrary unsteady conditions the use of the Steady State Global Equivalence Ratio Model (SSGERM) which has been proposed and supported by the two-layer steady-state data of Beyler (1986a, 1986b), Toner, Zukoski, and Kubota (1986), and Zukoski et al (1989 and 1991). Throughout this paper, these experiments and their data will be referred to as the SSGERM experiments and SSGERM data, respectively.

#### MODELING THE COMBUSTION PROCESS AND THE UNSTEADY ACCUMULATION OF MASS AND SPECIES IN THE EXTENDED UPPER LAYER

##### Two Components of the Model

Depicted in Figure 2 is a process diagram for the GGERM. The model involves two interacting components, a reactor and an accumulator. These two components interact by way of a feedback loop which passes material, at a rate to be determined, from the generally unsteady, but spatially-uniform-property accumulator to the input stream of the quasi-steady reactor.

##### Modeling the Combustion Process - The Reactor

In the phenomena being simulated, combustion processes are confined to a well-mixed volume of the extended upper layer. Depending on a variety of factors, at one extreme this combustion zone can be negligibly small and at the other can even dominate the entire layer. For example, in a Figure 1-type of fire scenario, combustion is often confined to the lower portion of the relatively small-volume, turbulent fire plume. Sometimes a fire can grow to the point that combustion even extends beyond the fire-plume volume and into a significant portion of the relatively small-volume, turbulent ceiling jet, the latter being formed by impingement of the burning plume on the ceiling surface. Under fuel rich conditions the combustion can fill most of the upper layer which itself can nearly fill the entire room.

The flow rates through the well-mixed combustion zone lead typically to characteristic residence times there which are small compared to the characteristic times of interest of the overall phenomena being modeled, but large compared to characteristic times of the combustion kinetics. This is the basis for modeling as quasi-steady the combustion processes.

All combustion processes are modeled by the reactor.

It is noteworthy that the reactor component of the model has a strong conceptual aspect in the sense that it is not intended to correspond strictly to any physical subdivision of the extended upper layer. Thus, while the role of the reactor is to simulate all significant combustion processes, there is no accounting

for the physical boundaries that would approximate the spatial limits of the combustion processes. For example, no material or material properties are directly associated with the "inside" of the reactor component, only material that enters and leaves it, and products of combustion that are generated by its action.

At least one aspect of the conceptual character of the reactor is highlighted in the model representation of Figure 2. As seen there, in the present model all flows entering the extended upper layer, pass through the reactor prior to being deposited in the accumulator. Yet, in the generic fire scenario depicted in Figure 1, it is clear that flows entering the upper layer from vents, e.g., from the doorway on the right side of the figure, do not enter directly a physical region of the extended upper layer that in any significant sense can be construed as the region wherein the significant combustion processes are taking place.

### Modeling the Bulk of the Upper Layer - The Accumulator

As observed in room fires, it is reasonable to model the properties of the major portion of the extended upper-layer volume as spatially uniform. This is modeled by the accumulator.

As indicated in Figure 2, instantaneous contents of the extended upper layer are assumed to reside in the accumulator, the average concentrations of products there being

$$c_{k,u} = P_{k,u}/m_u \quad (3)$$

Throughout the rest of this work, the  $P_{k,u}$  and  $c_{k,u}$  will correspond to the mass and mass fraction, respectively, of product  $k$  in the upper layer of a room of fire origin.

The SSGERM data were acquired under conditions of steady state. For this reason, an accumulator used in the modeling of those particular data would also be in a steady state. However, because the characteristic times for flows to pass through extended upper layers are typically relatively large, the properties of the accumulator in the model must be described generally as unsteady. In other words, the instantaneous rates of accumulation of products in the accumulator must be modeled as being generally non-zero and significant. The latter would be true even at times when the volume itself is relatively constant. As will be seen, such times of constant volume are exemplified by the transient upper layer environments in the experiments of Toner, Zukoski, and Kubota (1986) and Zukoski et al (1989 and 1991), where these transients lead to the steady state conditions reported.

Unlike the reactor, the physical boundaries of the accumulator are well-defined, namely, they are well-approximated by the boundaries of the upper layer. Yet, as with the reactor, aspects of the accumulator component of the present model must also be regarded as conceptual. For example, as noted before in Figure 2, any vent flows that are deposited into the upper layer are modeled as entering the reactor (i.e., the combustion process) prior to actually flowing into and mixing with the bulk of the upper layer. Again this is clearly in difference to the physical picture depicted in Figure 1. The conceptual character of the accumulator is also related to the fact that it is assumed to interact directly with the reactor. Thus, a model component (the accumulator) which interacts with a conceptual model component (the reactor) must itself be regarded as conceptual.

### The Flow Exchanges Between the Reactor and the Accumulator; the Flow-Rate in the Feedback Loop

Depicted in Figure 2 are the components of flow to the extended upper layer and flow exchanges between the reactor and the accumulator.

In general, the net flow to the extended upper layer is made up of a series of unidirectional flow components, flow components into the layer and flow components out of the layer. As indicated in Figure 2, the sum of all flow components of product  $k$  into the layer is designated as  $\dot{P}_{k, \text{FLOWIN}}$  and the sum of all flow components out of the layer is designated as  $\dot{P}_{k, \text{FLOWOUT}}$ . The  $\dot{P}_{k, \text{FLOWIN}}$  are all modeled as flowing directly to the input of the reactor prior to entering the accumulator.

The combustion process in the reactor leads to mass-generation-rate source terms for the products  $k$ . These are designated by  $\dot{\omega}_k$ . Conservation of mass requires that the sum of all  $\dot{\omega}_k$  is zero.

In view of the above, the  $\dot{P}_{k,u}$  of Eq. (1) are

$$\dot{P}_{k,u} = \dot{P}_{k, \text{FLOWIN}} - \dot{P}_{k, \text{FLOWOUT}} + \dot{\omega}_k \quad (4)$$

All  $\dot{P}_{k, \text{FLOWOUT}}$  are assumed to flow directly out of the extended upper layer from the accumulator, i.e., from the bulk of the upper layer. For example, in the fire scenario of Figure 1, the  $\dot{P}_{k, \text{FLOWOUT}}$  have two components. One of these is the flow of the products in the stream which passes from the upper layer in the room of fire origin through the upper vent in the wall on the right side to the adjacent space. The other components of  $\dot{P}_{k, \text{FLOWOUT}}$  are convected in the flow which is entrained into the relatively cool stream flowing into the fire room from the vent in the left wall. Because of its negative local buoyancy, this stream, together with the entrained material from the upper layer, flows downward and is deposited into the lower layer.

The  $\dot{P}_{k, \text{FLOWIN}}$  are made up of the sums of all types of inflow components. These include contributions of products of combustion  $k$  entrained from the lower layer into the plume, supplied directly from the fuel source, and flowing into the layer from wall, ceiling, or floor vents. The sketch of the fire scenario of Figure 1 indicates one vent flow stream which contributes to the  $\dot{P}_{k, \text{FLOWIN}}$ . This is the stream flowing across the layer interface on the right and entering the upper layer. This stream is driven by the locally upward-buoyancy of the flow through the doorway on the right.

As indicated in Figure 2, the inflow to the reactor is made up of the net flow rates,  $\dot{P}_{k, \text{REACTIN}}$  and their corresponding total mass flow rate,  $\dot{m}_{\text{REACTIN}}$ . The combustion processes in the reactor lead to the mass-generation-rate source terms,  $\dot{\omega}_k$ , which are depicted in the figures as separate inflows to the reactor (Figure 3) and to the overall extended upper layer (Figure 2).

For a given  $k$ ,  $\dot{P}_{k, \text{REACTIN}}$  has two components,  $\dot{P}_{k, \text{FLOWIN}}$  and  $\dot{P}_{k, \text{FEEDBK}}$ .

$$\dot{P}_{k, \text{REACTIN}} = \dot{P}_{k, \text{FLOWIN}} + \dot{P}_{k, \text{FEEDBK}} \quad (5)$$

$\dot{P}_{k, \text{FEEDBK}}$  is modeled as a product  $k$  flow rate introduced into the combustion process from the accumulator. This is represented by the feedback loop of Figure 2. The  $\dot{P}_{k, \text{FEEDBK}}$  and their corresponding total mass flow rate,  $\dot{m}_{\text{FEEDBK}}$ , can be thought of as representing a portion of the flow entrained into the combustion zone from the bulk of the upper layer. This

portion of flow will always have an effect on the combustion process by modifying the  $\omega_k$ 's.

As will be seen, a critical task in modeling the combustion process involves the establishment of model equations for  $\dot{m}_{\text{FEEDBK}}$  which are consistent with the SSGERM and with an arbitrary, unsteady, and fully-general two-layer zone-type description of a fire room environment.

As indicated in Figure 2, the reactor output,  $\dot{P}_{k, \text{REACTOUT}}$ , flows directly into the accumulator.

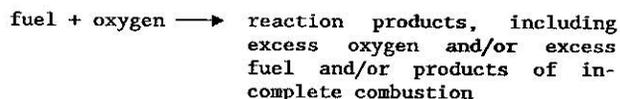
#### PREVIOUSLY ACQUIRED STEADY-STATE DATA, THE GLOBAL EQUIVALENCE RATIO, AND THE REACTOR COMBUSTION PROCESS

##### The Reactor Inflow and Outflow

The GGERM and SSGERM involve identical combustion models, i.e., relationships between reactor output and reactor input are the same for both.

##### A Model for the Reactor

Represent the reaction for a particular fuel by



Also, assume that the chemical composition of the fuel volatiles are known. Then for continuous idealized stoichiometric combustion of the fuel, it would be possible to calculate

$$r = (\dot{P}_{\text{FUEL}}/\dot{P}_{\text{OXY}})_{\text{STOICH}} \quad (6)$$

Here, idealized stoichiometric reactions of C, H, O-types of fuels refer to reactions where fuel and oxygen are mixed in proportions that ideally would lead only to  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , with no excess fuel or oxygen. It is assumed that  $r$  is known for a fuel of interest.

Define the global equivalence ratio,  $\phi$ , by

$$\phi = (\dot{P}_{\text{FUEL, REACTIN}}/\dot{P}_{\text{OXY, REACTIN}})/r \quad (7)$$

This is equivalent to the  $\phi$ -definitions used in the SSGERM experiments.

Since the combustion is assumed to be quasi-steady, i.e., no accumulation of products in the reactor,

$$\dot{P}_{k, \text{REACTOUT}} = \dot{P}_{k, \text{REACTIN}} + \omega_k \quad (8)$$

Note that for oxygen and fuel, which are consumed by the combustion,  $\omega_k$  would be negative. Inert flow components like  $\text{N}_2$  would be associated with  $\omega_k = 0$ .

As established in the SSGERM experiments

$$\omega_k/\dot{P}_{\text{FUEL, REACTIN}} = f_k(\phi) \quad (9)$$

Results reported by Zukoski et al (1991) indicate that the  $f_k$ 's are also generally functions of temperature, the dependency becoming important only for upper layer temperatures which exceed 800-900 K. For now this dependence will be ignored. Note that relative to the nomenclature of previous work, the  $f_k$  of Eq. (9) are identical to the "un-normalized yields" of Beyler (1986a, 1986b).

In principle one would hope that Eq. (9) is applicable to many practical fuels and that a standard test method could be established to determine for a particular fuel the  $f_k$  functions for all product  $k$ 's of interest. It is assumed that data to determine all such  $f_k$  functions for a fuel of interest have been acquired.

For the case of complete stoichiometric combustion, Eqs. (7)-(9) lead to

$$f_{\text{OXY}}^{\text{(STOICH)}} = \begin{cases} -1/r & \text{if } 0 \leq \phi \leq 1 \\ -1/(r\phi) & \text{if } \phi > 1 \end{cases} \quad (10)$$

$$f_{\text{FUEL}}^{\text{(STOICH)}} = \begin{cases} -1 & \text{if } 0 \leq \phi \leq 1 \\ -1/\phi & \text{if } \phi > 1 \end{cases} \quad (11)$$

Here, complete stoichiometric combustion means that: for fuel-lean inputs to the reactor, i.e.,  $0 \leq \phi \leq 1$ , all input fuel is consumed in an idealized stoichiometric reaction with the input oxygen; for fuel-rich inputs to the reactor, i.e.,  $\phi > 1$ , all input oxygen is consumed in an idealized stoichiometric reaction with the input fuel.

If all of the  $\dot{P}_{k, \text{REACTIN}}$  are known at a particular instant of time, then  $\phi$  can be calculated from Eq. (7),  $\omega_k$  can then be calculated from Eq. (9), and all components of the reactor output can be determined finally from Eq. (8).

Assume  $\dot{m}_{\text{REACTIN}}$  and the  $\dot{P}_{k, \text{REACTIN}}$  are known. Also, since the process "inside" the reactor is assumed to be quasi-steady,  $\dot{m}_{\text{REACTIN}} = \dot{m}_{\text{REACTOUT}}$ . Then, from Eqs. (8) and (9) the concentrations of the reactor outflow,  $c_{k, \text{REACTOUT}}$ , can be calculated from

$$c_{k, \text{REACTOUT}} = \quad (12)$$

$$[\dot{P}_{k, \text{REACTIN}} + \dot{P}_{\text{FUEL, REACTIN}} f_k(\phi)]/\dot{m}_{\text{REACTIN}}$$

Eq. (12) can also be expressed as

$$c_{k, \text{REACTOUT}} = \quad (13)$$

$$c_{\text{FUEL, REACTIN}} [\dot{P}_{k, \text{REACTIN}}/\dot{P}_{\text{FUEL, REACTIN}} + f_k(\phi)] \quad (13)$$

$$= c_{\text{OXY, REACTIN}} [\dot{P}_{k, \text{REACTIN}}/\dot{P}_{\text{OXY, REACTIN}} + \phi f_k(\phi)r] \quad (14)$$

With  $k \rightarrow$  fuel, Eq. (8) and Eq. (13) lead to

$$c_{\text{FUEL, REACTOUT}} = c_{\text{FUEL, REACTIN}} [1 + f_{\text{FUEL}}(\phi)] \quad (15)$$

With  $k \rightarrow$  oxygen, Eq. (14) leads to

$$c_{\text{OXY, REACTOUT}} = c_{\text{OXY, REACTIN}} [1 + \phi f_{\text{OXY}}(\phi)r] \quad (16)$$

For complete stoichiometric combustion, Eqs. (10) and (11) in Eqs. (15) and (16), respectively, lead to

$$c_{\text{FUEL, REACTOUT, STOICH}} = \begin{cases} 0 & \text{if } 0 \leq \phi \leq 1 \\ (1 - 1/\phi)c_{\text{FUEL, REACTIN}} & \text{if } \phi < 1 \end{cases} \quad (17)$$

$$c_{\text{OXY, REACTOUT, STOICH}} = \begin{cases} (1 - \phi)c_{\text{OXY, REACTIN}} & \text{if } 0 \leq \phi \leq 1 \\ 0 & \text{if } 1 < \phi \end{cases} \quad (18)$$

**A Requirement for Consistency Between the Reactor Model and Steady State Data Previously Acquired in Two-Layer Fire Experiments**

The SSGERM experiments involved burning in a standard atmosphere below the upper layer. The configuration used by Toner, Zukoski, and Kubota (1986) was similar to that used by Beyler (1986a, 1986b). Both are depicted in Figure 4. The work of Toner, Zukoski,

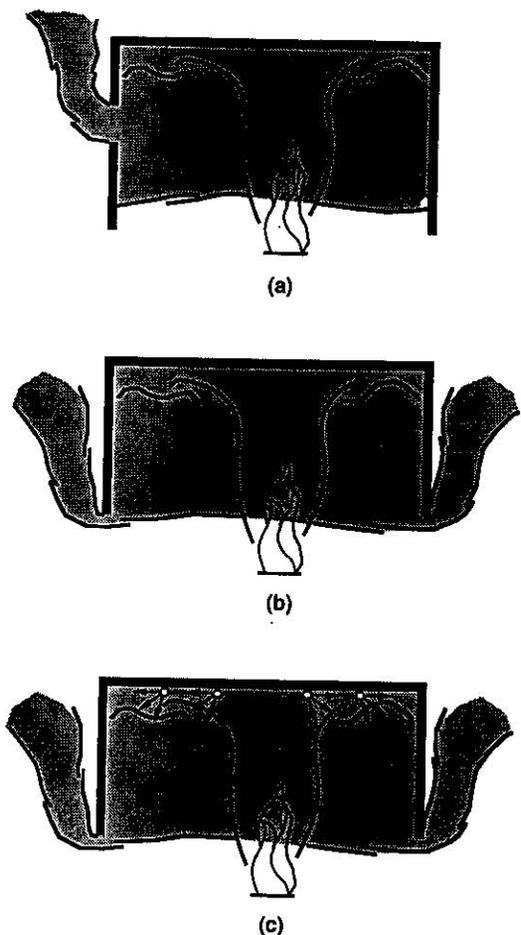


Fig. 4. The experimental configuration used by Beyler (1986a, 1986b) (a); Toner, Zukoski, and Kubota (1986) (b); and Zukoski et al (1989, 1991) (c).

and Kubota (1986) involved an inverted collector with contents "pouring out" below its bottom edge (Figure 4b). The work of Beyler (1986a, 1986b) involved a similar inverted collector, but with side venting and with the layer contained fully within the vessel (Figure 4a). For the purpose of the present analysis, the two configurations do not involve significant differences.

Also depicted in Figure 4c is the configuration used by Zukoski et al (1989, 1991). This is identical to that used by Toner, Zukoski, and Kubota (1986) except for the fact that here a steady flow of air was injected into the layer from many small holes near the top of the collector. This was done in a manner as to insure rapid

mixing between the injected air and the the flow produced by the fire plume.

The SSGERM data were reported for steady state conditions only. These are the data which were used to establish and validate the SSGERM and which will be used in the present GGERM.

The reactor model with the feedback-loop feature of Figure 2 will be seen to be generally consistent with the analyses of the SSGERM data if, at steady state, the feedback flow is identically zero. Thus, with zero feedback to the reactor, it is clear from Figure 2 that the steady stream of combustion products at the reactor output would flow, as in the SSGERM, without further reaction or alteration in concentration into and through the steady state accumulator.

Define  $\phi^{(SS)}$  and  $c_{k, \text{REACTOUT}}^{(SS)}$  as the values of  $\phi$  and  $c_{k, \text{REACTOUT}}$ , respectively, during a virtual steady state condition defined by the current inflow rates, but with zero flow in the feedback loop.

$$\phi^{(SS)} = (\dot{P}_{\text{FUEL, FLOWIN}} / \dot{P}_{\text{OXY, FLOWIN}}) / \tau \quad (19)$$

(Note  $\phi^{(SS)}$  is identical to  $\phi_2$  of Toner, Zukoski, and Kubota (1986), and Zukoski et al (1989, 1991) and to  $\phi$  of Beyler (1986a, 1986b). Then a criterion for consistency between the GGERM and SSGERM data is:

$$\begin{aligned} \text{When } c_{\text{FUEL, U}} &= c_{\text{FUEL, REACTOUT}}^{(SS)} \text{ and} \\ c_{\text{OXY, U}} &= c_{\text{OXY, REACTOUT}}^{(SS)} \text{ the GGERM should predict} \\ \dot{m}_{\text{FEEDBK}} &= \dot{m}_{\text{FEEDBK}} = 0. \end{aligned} \quad (20)$$

**THE FLOW FROM THE ACCUMULATOR TO THE REACTOR - A MODEL FOR  $\dot{m}_{\text{FEEDBK}}$**

**Considerations in the Establishment of the Feedback Flow Model**

The feedback flow rate model is based on the following considerations:

1. The proposed GGERM must be completely consistent with the SSGERM. This is guaranteed if a)  $\omega_k$  satisfies Eq. (9); and b) the feedback flow rate is identically zero under steady state conditions and satisfies the criterion of (20).
2. When the feedback flow rate is nonzero, it is reasonable to assume that it is an explicit function of upper layer oxygen and fuel concentration. The present "first-order" model assumes a continuous, piecewise-linear functional relationship of the form

$$\dot{m}_{\text{FEEDBK}} = \alpha_{\text{FUEL}} (c_{\text{FUEL, U}} - c_{\text{FUEL, REACTOUT}}^{(SS)}) + \alpha_{\text{OXY}} (c_{\text{OXY, U}} - c_{\text{OXY, REACTOUT}}^{(SS)})$$

where  $\dot{m}_{\text{FEEDBK}} \geq 0$ ,  $\alpha_{\text{FUEL}} \geq 0$ , and  $\alpha_{\text{OXY}} \geq 0$ .

3. When the oxygen concentration in the accumulator is equal to some maximum achievable value and fuel concentration in the accumulator is zero,  $\dot{m}_{\text{FEEDBK}}$  will be the minimum value that results in complete consumption of fuel in the reactor combustion process.
4. When the fuel concentration in the accumulator is equal to some maximum achievable value and oxygen concentration in the accumulator is zero,  $\dot{m}_{\text{FEEDBK}}$  will be the minimum value that results in complete

consumption of oxygen in the reactor combustion process.

Expressions for the  $c_{k,REACTOUT}^{(SS)}$  as functions of upper layer inflow will now be developed. These are required in the feedback flow model. The expressions will then be related to the SSGERM data. This section concludes with a presentation of the proposed  $m_{FEEDBK}$  equations which take into account all of the above considerations.

#### Definitions of $\phi_{FUEL}$ and $\phi_{OXY}$

Eqs. (12), (15), and (16) lead to

$$c_{k,REACTOUT}^{(SS)} = \frac{[\dot{P}_{k, FLOWIN} + \dot{P}_{FUEL, FLOWIN} f_k(\phi^{(SS)})]/m_{FLOWIN}}{c_{FUEL, FLOWIN} [1 + f_{FUEL}(\phi^{(SS)})]} \quad (21)$$

$$c_{FUEL, REACTOUT}^{(SS)} = c_{FUEL, FLOWIN} [1 + f_{FUEL}(\phi^{(SS)})] \quad (22)$$

$$c_{OXY, REACTOUT}^{(SS)} = c_{OXY, FLOWIN} [1 + \phi^{(SS)} f_{OXY}(\phi^{(SS)})r] \quad (23)$$

For a fuel of interest, define  $\phi_{FUEL}$  as the maximum value of  $\phi$  which leads to complete consumption of fuel, i.e., which leads to  $\dot{P}_{FUEL, REACTOUT} = 0$ . Using Eq. (8) and (9) with  $k \rightarrow$  fuel, it can be shown that  $\phi_{FUEL}$  satisfies

$$\phi_{FUEL} = \text{maximum root of } f_{FUEL}(\phi_{FUEL}) + 1 = 0 \quad (24)$$

Define similarly  $\phi_{OXY}$  as the minimum value of  $\phi$  which leads to complete consumption of oxygen, i.e., which leads to  $\dot{P}_{OXY, REACTOUT} = 0$ .

$$\phi_{OXY} = \text{minimum root of } \phi_{OXY} f_{OXY}(\phi_{OXY})r + 1 = 0 \quad (25)$$

For a combustion system involving complete stoichiometric combustion,  $\phi_{FUEL} = \phi_{OXY} = 1$  and, using Eqs. (10) and (11), Eqs. (22) and (23) become

$$c_{FUEL, REACTOUT, STOICH}^{(SS)} = \begin{cases} 0 & \text{if } 0 \leq \phi^{(SS)} \leq 1 \\ (1 - 1/\phi^{(SS)})c_{FUEL, FLOWIN} & \text{if } 1 < \phi^{(SS)} \end{cases} \quad (26)$$

$$c_{OXY, REACTOUT, STOICH}^{(SS)} = \begin{cases} (1 - \phi^{(SS)})c_{OXY, FLOWIN} & \text{if } 0 \leq \phi^{(SS)} \leq 1 \\ 0 & \text{if } 1 < \phi^{(SS)} \end{cases} \quad (27)$$

For real systems,  $0 < \phi_{FUEL} < 1 < \phi_{OXY}$ .

#### Steady State Concentrations and the SSGERM Experiments

Consider the SSGERM data for the  $c_{k,U}$ . Because of the steady state condition, these concentrations are identical to the  $c_{k,REACTOUT}^{(SS)}$  of Eqs. (21)-(23). Also, since flow to the upper layer is only from a "pure" fuel source and from air of a standard atmosphere, it is reasonable to assume that the  $\dot{P}_{k, FLOWIN}$  are negligible for all (non-inert) products  $k$  other than fuel and oxygen. Therefore, Eq. (21) can be written as

$$c_{k,REACTOUT}^{(SS)} = c_{FUEL, FLOWIN} f_k(\phi^{(SS)}) \quad (28)$$

k not fuel or oxygen

Also, using Eq. (19) and the fact that the mass fraction of oxygen in air is 0.232 it can be shown that

$$c_{FUEL, FLOWIN} = 0.232\phi^{(SS)}r/(1 + 0.232\phi^{(SS)}r) \quad (29)$$

$$c_{OXY, FLOWIN} = 0.232/(1 + 0.232\phi^{(SS)}r) \quad (30)$$

Finally, Eqs. (29) and (30) in Eqs. (22), (23), and (28) lead to

For SSGERM-type experiments:

$$c_{FUEL, REACTOUT}^{(SS)} = 0.232\phi^{(SS)}r[1 + f_{FUEL}(\phi^{(SS)})]/(1 + 0.232\phi^{(SS)}r) \quad (31)$$

$$c_{OXY, REACTOUT}^{(SS)} = 0.232[1 + \phi^{(SS)}f_{OXY}(\phi^{(SS)})r]/(1 + 0.232\phi^{(SS)}r) \quad (32)$$

$$c_{k, REACTOUT}^{(SS)} = 0.232\phi^{(SS)}f_k(\phi^{(SS)})r/(1 + 0.232\phi^{(SS)}r) \quad (33)$$

k not fuel or oxygen

It can be shown that fuel and oxygen concentrations for complete stoichiometric combustion, as given in Eqs. (17) and (18), respectively, are properly recovered when  $f_{OXY}^{(STOICH)}$  of Eq. (11) and  $f_{FUEL}^{(STOICH)}$  of Eq. (10) are used in Eqs. (31) and (32), respectively.

The results of Eqs. (31)-(33) reaffirm the consistency of the GGERM proposed here and the SSGERM as established in the SSGERM experiments. Thus, for given fuels, i.e., for fixed values of  $(\dot{P}_{FUEL}/\dot{P}_{OXY})_{STOICH}$ , the GGERM predicts that under steady state conditions the concentrations of any product of combustion  $k$  in the bulk of the upper layer is a function only of  $\phi^{(SS)}$  and  $f_k(\phi^{(SS)})$ . Given a SSGERM-type of experiment which uses a fuel with known  $r$ , steady state data in the form of a plot of  $c_{k,REACTOUT}^{(SS)}$  as a function of  $\phi^{(SS)}$  can therefore be used to obtain any of the  $f_k(\phi)$ .

To illustrate this, consider data presented by Zukoski et al (1991) which were obtained from experiments with natural gas. Assume the fuel to be pure methane,  $CH_4$ . Then the stoichiometric reaction is  $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$ , and it follows that

$$r = (\dot{P}_{CH_4}/\dot{P}_{OXY})_{STOICH} = 16/64 = 1/4 \quad (34)$$

For SSGERM experiments using methane, Eqs. (31)-(34) lead to:

$$c_{CH_4, REACTOUT}^{(SS)} = (0.232/4)\phi^{(SS)}[1 + f_{CH_4}(\phi^{(SS)})]/[1 + (0.232/4)\phi^{(SS)}] \quad (35)$$

$$c_{OXY, REACTOUT}^{(SS)} = 0.232[1 + (1/4)\phi^{(SS)}f_{OXY}(\phi^{(SS)})]/[1 + (0.232/4)\phi^{(SS)}] \quad (36)$$

$$c_{k, REACTOUT}^{(SS)} = (0.232/4)\phi^{(SS)}f_k(\phi^{(SS)})/[1 + (0.232/4)\phi^{(SS)}] \quad (37)$$

k not fuel or oxygen

The right hand sides of Eqs. (35)-(37) are used to provide additional labels on the data plots, presented in Figures 1-4 of Zukoski et al (1991) and reproduced here in Figures 5-8. These plots are for the steady state upper layer mass fractions of O<sub>2</sub>, CH<sub>4</sub>, CO, and H<sub>2</sub>, respectively, i.e., for the experimentally determined values of  $c_{k,REACTOUT}^{(SS)}$ . In Figures 5-8, it should be noted that the steady state data of Toner were acquired in experiments where temperatures were higher than 900 K (Zukoski et al, 1991). As stated below Eq. (9), the present model would not be expected to provide accurate predictions of these data. The Toner data in the plots of Figures 5-8 should be ignored from present consideration.

Note that for methane, Eq. (24) with Figure 5 and Eq. (25) with Figure 6 result in  $\phi_{CH_4} \approx 0.7$  and  $\phi_{O_2} \approx 3.0$ , respectively.

Consistent with the SSGERM, the relevant data of Figures 5-8 are all well-correlated, i.e., the measured  $c_{k,REACTOUT}^{(SS)}$  data can be approximated by curve-fit

functions  $c_{k,REACTOUT}^{(SS,FIT)}(\phi^{(SS)})$ . Using Eqs. (35)-(37), such curve fit functions could then be used to calculate the  $f_k$ 's for methane from:

For methane:

$$f_{CH_4}(\phi) = c_{CH_4,REACTOUT}^{(SS,FIT)}(\phi)[1 + (4/0.232)/\phi] - 1 \quad (35')$$

$$f_{O_2}(\phi) = c_{O_2,REACTOUT}^{(SS,FIT)}(\phi) + (4/\phi)[c_{O_2,REACTOUT}^{(SS,FIT)}(\phi)/0.232 - 1] \quad (36')$$

$$f_k(\phi) = c_{k,REACTOUT}^{(SS,FIT)}(\phi)[1 + (4/0.232)/\phi] \quad (37')$$

k not fuel or oxygen

Note that in Eqs. (35')-(37') the apparent singularities at  $\phi = 0$  can be removed when one takes note of the fact that  $c_{CO_2,REACTOUT}^{(SS,FIT)}(0) = 0.232$  and  $c_{k,REACTOUT}^{(SS,FIT)}(0) = 0$  for fuel and, as assumed here, for all other products in the experiments under consideration.

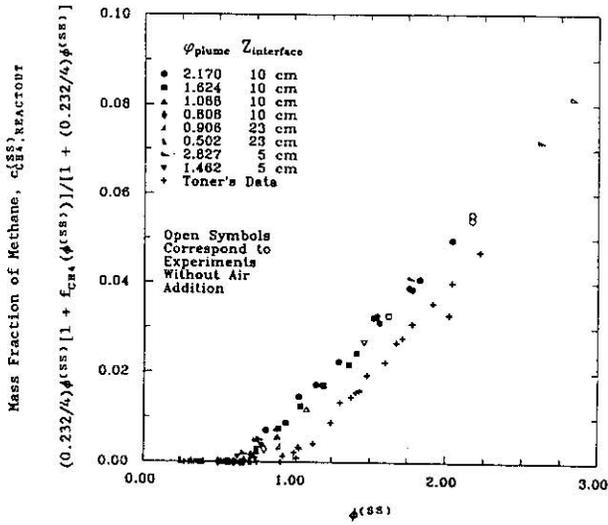


Fig. 5. Relabeled Figure 3 of Zukoski et al (1991) according to Eq. (35) for data of  $c_{CH_4,REACTOUT}^{(SS)}$ .

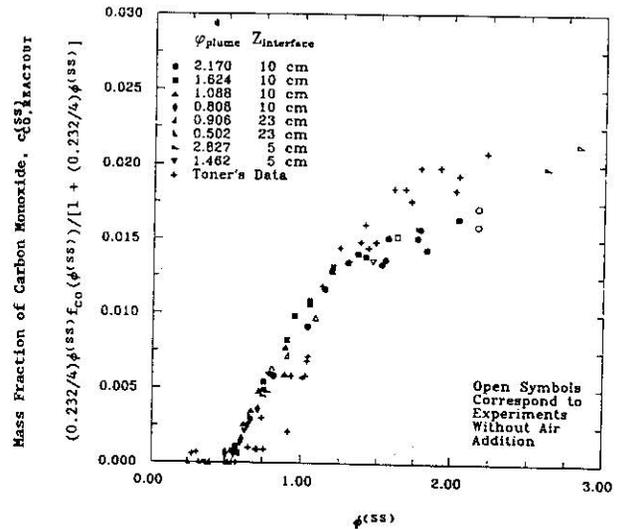


Fig. 7. Relabeled Figure 2 of Zukoski et al (1991) according to Eq. (37) for data of  $c_{CO,REACTOUT}^{(SS)}$ .

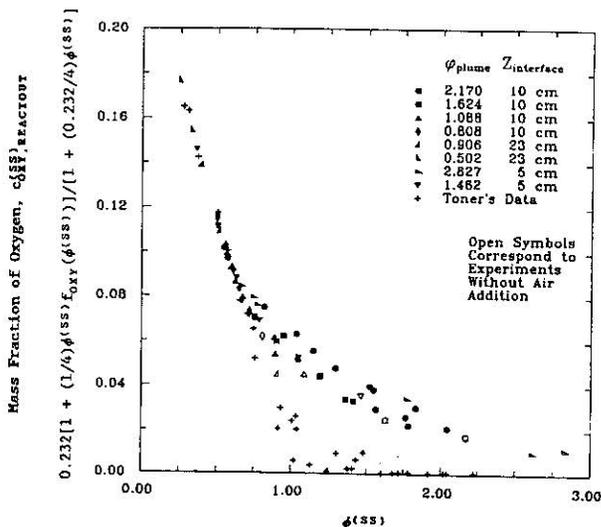


Fig. 6. Relabeled Fig. 1 of Zukoski et al (1991) according to Eq. (36) for data of  $c_{O_2,REACTOUT}^{(SS)}$ .

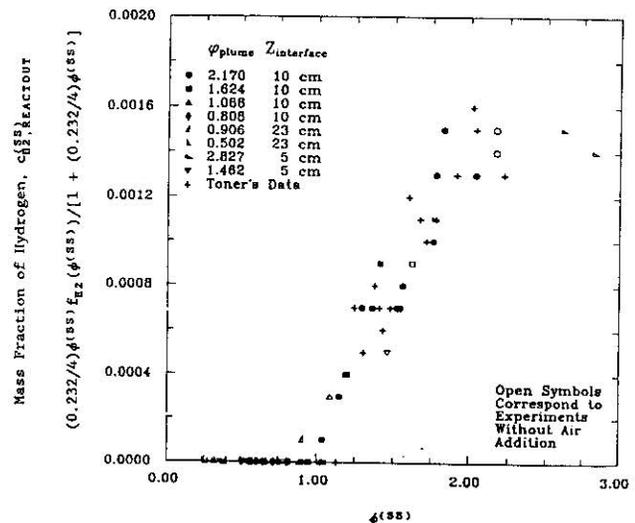


Fig. 8. Relabeled Figure 4 of Zukoski et al (1991) according to Eq. (37) for data of  $c_{H_2,REACTOUT}^{(SS)}$ .

### The Model for $m_{FEEDBK}$

A model for  $m_{FEEDBK}$  is now presented which satisfies all considerations outlined at the beginning of this section. Three possible cases are considered: Case 1:  $c_{OXY,U} \geq 0$ ,  $c_{FUEL,U} = 0$ ; Case 2:  $c_{OXY,U} \geq 0$ ,  $c_{FUEL,U} \geq 0$ ; and Case 3:  $c_{OXY,U} = 0$ ,  $c_{FUEL,U} \geq 0$ .

Case 1:  $c_{OXY,U} \geq 0$ ,  $c_{FUEL,U} = 0$

Here take  $m_{FEEDBK} = m_{FEEDBK,1}$  (subscript 1 is for Case 1) as proportional to  $c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)}$ , if  $c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)} \geq 0$ , and take  $m_{FEEDBK} = 0$  if  $c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)} < 0$ . Thus, provided  $\phi^{(SS)} \geq \phi_{FUEL}$ , it is assumed that a relatively high concentration of oxygen in the upper layer (i.e., compared to the concentration in the virtual steady state) will enhance combustion in the reactor leading to  $c_{OXY,REACTOUT} > c_{OXY,REACTOUT}^{(SS)}$ , while a relatively low concentration of oxygen in the layer will not generally affect the combustion at all. Note that in the latter situation, where feedback is zero, the  $c_{OXY,U}$  of the layer will tend to be increased by the relatively rich oxygen concentration of the reactor output,  $c_{OXY,REACTOUT}^{(SS)}$ , but that this will occur by a simple mixing process.

$$m_{FEEDBK,1} = \begin{cases} m_{FEEDBK}^{(1)} (c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)}) / \\ (c_{OXY,U}^{(MAX)} - c_{OXY,REACTOUT}^{(SS)}) & \text{if } c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)} \geq 0 \\ 0 & \text{if } (c_{OXY,U} - c_{OXY,REACTOUT}^{(SS)}) < 0 \end{cases} \quad (38)$$

where  $c_{OXY,U}^{(MAX)}$  is the maximum possible value of  $c_{OXY,U}$ , taken to be 0.232, and where  $m_{FEEDBK}^{(1)}$ , the characteristic value of  $m_{FEEDBK,1}$ , is taken to be the minimum feedback mass flow-rate from a  $c_{OXY,U}^{(MAX)}$  upper layer environment to the reactor input stream which, together with the  $\dot{P}_{OXY,FLOWIN}$  oxygen flow rate, would consume completely the  $\dot{P}_{FUEL,FLOWIN}$  fuel flow rate. Thus, for  $\phi^{(SS)} \leq \phi_{FUEL}$  (no fuel in the reactor output stream under zero feedback conditions),  $m_{FEEDBK}^{(1)} = 0$ , while for  $\phi^{(SS)} \geq \phi_{FUEL}$ , the combined flow rate of oxygen,  $m_{FEEDBK}^{(1)} c_{OXY,U}^{(MAX)} + \dot{P}_{OXY,FLOWIN}$ , and flow rate of fuel,  $\dot{P}_{FUEL,FLOWIN}$ , to the reactor input leads, by definition, to  $\phi = \phi_{FUEL}$ , i.e.,

$$\phi_{FUEL} = [\dot{P}_{FUEL,FLOWIN} / (m_{FEEDBK}^{(1)} c_{OXY,U}^{(MAX)} + \dot{P}_{OXY,FLOWIN})] / r \quad (39)$$

Solving Eq. (39) for  $m_{FEEDBK}^{(1)}$

$$m_{FEEDBK}^{(1)} = \begin{cases} 0 & \text{if } \phi^{(SS)} / \phi_{FUEL} \leq 1 \\ (1 - \phi_{FUEL} / \phi^{(SS)}) \dot{P}_{FUEL,FLOWIN} / (c_{OXY,U}^{(MAX)} \phi_{FUEL} r) & \text{if } \phi^{(SS)} / \phi_{FUEL} > 1 \end{cases} \quad (40)$$

For complete stoichiometric reactions Eqs. (38) and (40) become

$$m_{FEEDBK,1,STOICH} = \begin{cases} 0 & \text{if } 0 \leq \phi^{(SS)} \leq 1 \\ (1 - 1/\phi^{(SS)}) (c_{OXY,U} / c_{OXY,U}^{(MAX)}) \cdot \dot{P}_{FUEL,FLOWIN} / (c_{OXY,U}^{(MAX)} r) & \text{if } 1 < \phi^{(SS)} \end{cases} \quad (41)$$

An example of a Case-1 fire scenario is one where the upper layer has an environment of near-normal atmospheric oxygen concentration and negligible fuel, i.e.,  $c_{OXY,U} \approx 0.232$  and  $c_{FUEL,U} \approx 0$ . For such scenarios,  $\phi^{(SS)}$  can range from values close to 0, e.g., relatively large entrainment of air (oxygen) into the portion of the plume below the layer interface, to arbitrarily large values, e.g., no oxygen enters the layer from below the interface. The latter situation would correspond to a case where the fuel source is actually submerged in the upper layer, e.g. as in the configuration in Figure 4b. An analysis of this example will be presented below.

It is convenient to consider Case 3 before Case 2.

Case 3:  $c_{OXY,U} = 0$ ,  $c_{FUEL,U} \geq 0$

Here take  $m_{FEEDBK} = m_{FEEDBK,3}$  (where subscript 3 is associated with Case 3) as proportional to  $c_{FUEL,U} - c_{FUEL,REACTOUT}^{(SS)}$ , if  $c_{FUEL,U} - c_{FUEL,REACTOUT}^{(SS)} \geq 0$ , and  $m_{FEEDBK} = 0$  if  $c_{FUEL,U} - c_{FUEL,REACTOUT}^{(SS)} < 0$ . Thus, provided  $\phi^{(SS)} < \phi_{OXY}$ , it is assumed that a relatively high concentration of fuel in the upper layer (i.e., compared to that in the virtual steady state) will enhance combustion in the reactor leading to  $c_{FUEL,REACTOUT} > c_{FUEL,REACTOUT}^{(SS)}$ , while a relatively low concentration of fuel in the layer will not generally affect the combustion at all. Note that in the latter situation, where feedback is zero, the low  $c_{FUEL,U}$  of the layer will tend to be increased by the relatively rich fuel concentration of the reactor output,  $c_{FUEL,REACTOUT}^{(SS)}$ , but that this will occur by a simple mixing process.

$$m_{FEEDBK,3} = \begin{cases} m_{FEEDBK}^{(3)} (c_{FUEL,U} - c_{FUEL,REACTOUT}^{(SS)}) / \\ (c_{FUEL,U}^{(MAX)} - c_{FUEL,REACTOUT}^{(SS)}) & \text{if } c_{FUEL,U} - c_{FUEL,REACTOUT}^{(SS)} \geq 0 \\ 0 & \text{if } c_{FUEL,U} - c_{FUEL,REACTOUT}^{(SS)} < 0 \end{cases} \quad (42)$$

where  $c_{FUEL,U}^{(MAX)}$  is the maximum possible value of  $c_{FUEL,U}$ , taken to be 1, and where  $m_{FEEDBK}^{(3)}$ , the characteristic value of  $m_{FEEDBK,3}$ , is taken to be the minimum feedback mass flow rate from a  $c_{FUEL,U}^{(MAX)}$  upper layer environment to the reactor input stream which, together with the  $\dot{P}_{FUEL,FLOWIN}$  fuel flow rate, would consume completely the  $\dot{P}_{OXY,FLOWIN}$  oxygen flow rate. Thus, for  $\phi^{(SS)} \geq \phi_{OXY}$  (no oxygen in the reactor output stream under zero feedback conditions),  $m_{FEEDBK}^{(3)} = 0$ , while for  $\phi^{(SS)} < \phi_{OXY}$ , the combined fuel flow rate,  $m_{FEEDBK}^{(3)} c_{FUEL,U}^{(MAX)} + \dot{P}_{FUEL,FLOWIN}$ , and oxygen flow rate,  $\dot{P}_{OXY,FLOWIN}$ , to the reactor input leads, by definition, to  $\phi = \phi_{OXY}$ , i.e.,

$$\phi_{OXY} = [(\dot{P}_{FUEL,FLOWIN} + m_{FEEDBK}^{(3)} c_{FUEL,U}^{(MAX)}) / \dot{P}_{OXY,FLOWIN}] / r \quad (43)$$

Solving for  $m_{FEEDBK}^{(3)}$

$$m_{FEEDBK}^{(3)} = \begin{cases} 0 & \text{if } \phi_{OXY} / \phi^{(SS)} \leq 1 \\ (1 - \phi^{(SS)} / \phi_{OXY}) \dot{P}_{OXY,FLOWIN} \phi_{OXY} r / c_{FUEL,U}^{(MAX)} & \text{if } \phi_{OXY} / \phi^{(SS)} > 1 \end{cases} \quad (44)$$

For complete stoichiometric reactions Eqs. (42) and (44) become

$\dot{m}_{FEEDBK,3,STOICH} -$

(45)

$$\left\{ \begin{array}{l} (1 - \phi^{(SS)})(c_{FUEL,U}/c_{FUEL,U}^{(MAX)}) \\ \dot{P}_{OXY, FLOWIN} \tau / c_{FUEL,U}^{(MAX)} \text{ if } 0 \leq \phi^{(SS)} \leq 1 \\ 0 \text{ if } 1 < \phi^{(SS)} \end{array} \right.$$

An example of a Case-3 fire scenario is one where the upper layer is established with an environment of pure fuel, i.e.,  $c_{OXY,U} \approx 0$  and  $c_{FUEL,U} \approx 1$ . Then, if  $\phi^{(SS)} < \phi_{OXY}$  and if a burning fuel source is located below the layer interface, some oxygen introduced into the upper layer would react with the upper-layer fuel. Note that here a  $\phi^{(SS)} = 0$  condition can be established if a source of oxygen (and an initial ignitor) is submerged completely in the upper layer.

The latter example involves an idealized scenario in that  $c_{FUEL,U} \approx 1$  would not occur in a typical situation where the room containing the fire has a non-zero lower layer with a non-zero concentration of oxygen. This is the case since, as the fuel concentration in the upper layer increased from zero, ignition and burning at the layer interface and in the layer itself would occur at a characteristic fuel concentration significantly less than 1 (Beyler, 1984). Ignition criteria for initiation of such layer burning would be determined from the known concentrations of oxygen and combustible species in the layers.

Case 2:  $c_{OXY,U} \geq 0$ ,  $c_{FUEL,U} \geq 0$

For this case,  $\dot{m}_{FEEDBK} = \dot{m}_{FEEDBK,2}$  is taken to be

$$\dot{m}_{FEEDBK,2} = \max(\dot{m}_{FEEDBK,1}, \dot{m}_{FEEDBK,3}) \quad (46)$$

All Cases:

Noting that Eq. (46) reduces to Eq. (38) or (41) if  $c_{FUEL,U} = 0$  and that Eq. (46) reduces to Eq. (42) or (45) if  $c_{OXY,U} = 0$ , it is evident that Eq. (46) predicts  $\dot{m}_{FEEDBK}$  uniformly for every possible fire scenario, i.e., for all cases 1, 2, and 3. It is therefore concluded that in general

$$\dot{m}_{FEEDBK} = \max(\dot{m}_{FEEDBK,1}, \dot{m}_{FEEDBK,3}) \quad (47)$$

where  $\dot{m}_{FEEDBK,1}$  and  $\dot{m}_{FEEDBK,3}$  are computed from Eqs. (38) or (41) and (42) or (45), respectively.

**AN ALGORITHM FOR INVOKING CONSERVATION OF PRODUCTS OF COMBUSTION IN THE UPPER LAYER OF A ROOM CONTAINING A FIRE**

Consider the extended upper layer of a room of fire origin where  $\dot{P}_{k, FLOWIN}$  and  $\dot{P}_{k, FLOWOUT}$  of Eq. (4) are assumed to be available. Completion of the right side of Eq. (1) and integration to the next time step requires an estimate for the generally unknown  $\omega_k$ 's. The following is the proposed procedure for obtaining such an estimate:

1. Determine  $\phi^{(SS)}$  from Eq. (22).
2. Determine  $\dot{m}_{FEEDBK}$  from Eq. (49).
3. From the known  $c_{k,U}$ , determine the  $\dot{P}_{k, FEEDBK} = \dot{m}_{FEEDBK} c_{k,U}$  and use these in Eq. (5) with the known  $\dot{P}_{k, FLOWIN}$  to determine the  $\dot{P}_{k, REACTIN}$ .
4. With the now-known  $\dot{P}_{FUEL, REACTIN}$  and  $\dot{P}_{OXY, REACTIN}$ , determine  $\phi$  from Eq. (7) and then the  $\omega_k$ 's from Eq. (9).

**PREDICTING  $c_{k,U}$  IN THE SSGERM EXPERIMENTS FROM THE INITIAL CONDITIONS TO STEADY STATE - AN EXAMPLE APPLICATION OF THE GGERM**

The Initial Value Problem for the  $c_{k,U}$

Use of the GGERM will now be illustrated by setting up the problem and solving for the history of the  $c_{k,U}$  in the SSGERM experiments.

Assume: 1) the upper-layer volume,  $V$ , is fixed at the volume of the collector and is initially pure air, i.e., no non-inert components except for oxygen with a mass fraction of 0.232 [this assumption would not be valid in the experiments of Beyler (1986a, 1986b)]; 2) net rates of inflow of fuel, oxygen, and inerts to the upper layer are constant and specified, and rates of inflow of all other products of combustion are negligible [see the discussion above Eq. (8)]; 3) the upper layer can be reasonably modeled as an ideal gas where properties are identical to those of air and the absolute pressure is well-approximated by  $p_{ATM}$ , a characteristic pressure of the ambient; 4) the temperature history,  $T_U(t)$ , of the upper layer is known, and  $T_U(0) = T_{AMB}$ , the temperature of the laboratory; and 5) for the fuel being burned, the  $f_k(\phi)$  for all products of interest are known.

Eqs. (1) and (3) lead to

$$\dot{m}_U dc_{k,U} / dt = (c_{k, REACTOUT} - c_{k,U})(\dot{m}_{FLOWIN} + \dot{m}_{FEEDBK}) \quad (48)$$

The problem for  $c_{FUEL,U}$  and  $c_{OXY,U}$ . For  $k \rightarrow$  fuel or oxygen, it can be shown from Eqs. (15) and (16) that Eq. (48) can be written as

$$\dot{m}_U dc_{FUEL,U} / dt = \quad (49)$$

$$c_{FUEL,U} \dot{m}_{FEEDBK} f_{FUEL}(\phi) - c_{FUEL,U} \dot{m}_{FLOWIN} + \dot{P}_{FUEL, FLOWIN} [1 + f_{FUEL}(\phi)]$$

$$\dot{m}_U dc_{OXY,U} / dt = \quad (50)$$

$$c_{OXY,U} \dot{m}_{FEEDBK} \phi f_{OXY}(\phi) \tau - c_{OXY,U} \dot{m}_{FLOWIN} + \dot{P}_{OXY, FLOWIN} [1 + \phi f_{OXY}(\phi) \tau]$$

$$\phi = [(\dot{P}_{FUEL, FLOWIN} + c_{FUEL,U} \dot{m}_{FEEDBK}) / \quad (51)$$

$$(\dot{P}_{OXY, FLOWIN} + c_{OXY,U} \dot{m}_{FEEDBK})] / \tau$$

$$\dot{m}_{FEEDBK} = \quad (52)$$

$$\dot{m}_{FEEDBK}(\text{inflow conditions}, c_{FUEL,U}, c_{OXY,U})$$

where  $\dot{m}_{FEEDBK}$  of Eq. (52) is determined from Eq. (47).

The equation of state for the upper layer leads to

$$\dot{m}_U = V \rho_U = V p_{AMB} / (RT_U) \quad (53)$$

where  $\rho_U$  is the density of the upper layer and  $R$  is the gas constant for air. Then Eq. (53) and the known data on  $T_U(t)$  yield an estimate for  $\dot{m}_U(t)$ .

Eqs. (49) and (50) determine  $c_{FUEL,U}$  and  $c_{OXY,U}$  from  $t = 0$  to steady state. To solve these, subject to the initial conditions

$$c_{FUEL,U}(t = 0) = 0; \quad c_{OXY,U}(t = 0) = c_{OXY,U}^{(MAX)} = 0.232 \quad (54)$$

the right hand sides would be determined from Eqs. (51) and (52) and from the assumed known functions  $f_{\text{FUEL}}(\phi)$  and  $f_{\text{OXY}}(\phi)$  for the fuel of interest.

The problem for  $c_{k,U}$  for k not fuel or oxygen. Consistent with assumption 2,

$$\dot{P}_{k, \text{FLOWIN}} = 0 \text{ for } k \text{ other than fuel or oxygen} \quad (55)$$

Using Eqs. (55), (13), and (14) in Eq. (48) it can be shown that the initial value problems for the  $c_{k,U}$  can be written in any of the following forms

for k not fuel or oxygen:

$$m_U dc_{k,U}/dt + c_{k,U} \dot{m}_{\text{FLOWIN}} = (c_{\text{FUEL},U} \dot{m}_{\text{FEEDBK}} + \dot{P}_{\text{FUEL},\text{FLOWIN}}) f_k(\phi) \quad (56)$$

$$= (c_{\text{OXY},U} \dot{m}_{\text{FEEDBK}} + \dot{P}_{\text{OXY},\text{FLOWIN}}) \phi f_k(\phi) \quad (57)$$

$$- \lambda_k(t) \quad (58)$$

$$c_{k,U}(t=0) = 0 \quad (59)$$

Once the solutions of Eqs. (49)-(54) for  $c_{\text{FUEL},U}$  and  $c_{\text{OXY},U}$  have been obtained, the  $\lambda_k(t)$  of Eq. (58) are known.  $c_{k,U}$ , for other products of interest would then be obtained from solutions of Eqs. (58) and (59).

Solution for the  $c_{k,U}$  Assuming Complete Stoichiometric Combustion

The functions  $f_k(\phi)$  for k not fuel or oxygen. Assume complete stoichiometric combustion. Then, excess fuel or excess oxygen brought into the reactor would lead to  $\phi > 1$  or  $\phi < 1$ , respectively, and to excess fuel or oxygen at the reactor output.

As an example, assume that the fuel is  $\text{CH}_4$ , where the reaction is presented above Eq. (34). Then for k →  $\text{CO}_2$  or  $\text{H}_2\text{O}$  and for excess oxygen to the reactor, i.e., for  $\phi < 1$ , the rate of generation of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  in the combustion is determined by the rate of supply of fuel to the reactor. Similarly, for excess fuel to the reactor, i.e.,  $\phi > 1$ , the rate of generation of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  is determined by the rate of supply of oxygen. Eqs. (7)-(9) and (34) lead to

For complete stoichiometric combustion of  $\text{CH}_4$ :

$$f_{\text{CO}_2}^{(\text{STOICH})} = \begin{cases} 11/4 & \text{if } 0 \leq \phi \leq 1 \\ (11/4)/\phi & \text{if } \phi > 1 \end{cases} \quad (60)$$

$$f_{\text{H}_2\text{O}}^{(\text{STOICH})} = \begin{cases} 9/4 & \text{if } 0 \leq \phi \leq 1 \\ (9/4)/\phi & \text{if } \phi > 1 \end{cases}$$

It is noted that for the complete stoichiometric combustion of any fuel and for any k, the  $f_k^{(\text{STOICH})}(\phi)$  would have the identical form as that displayed above for methane, i.e.,

For complete stoichiometric combustion of any fuel and for any k:

$$f_k^{(\text{STOICH})} = \begin{cases} C_k & \text{if } 0 \leq \phi \leq 1 \\ C_k/\phi & \text{if } \phi > 1 \end{cases} \quad (61)$$

where the  $C_k$  are constants determined by the stoichiometric reaction. For k → fuel and oxygen,  $C_{\text{FUEL}} = -1$  and

$C_{\text{OXY}} = -1/(\dot{P}_{\text{CH}_4}/\dot{P}_{\text{OXY}})_{\text{STOICH}}$ , respectively, have already been presented in Eqs. (10) and (11).

Solutions for the  $c_{k,U}$ . Since complete stoichiometric combustion is assumed, Eqs. (17) and (18) can be used in Eq. (48), or Eqs. (10) and (11) in Eqs. (49) and (50). This leads to

If  $0 \leq \phi \leq 1$ :

$$m_U dc_{\text{FUEL},U}/dt = -c_{\text{FUEL},U} (\dot{m}_{\text{FEEDBK}} + \dot{m}_{\text{FLOWIN}}) \quad (62)$$

$$m_U dc_{\text{OXY},U}/dt = -c_{\text{OXY},U} (\phi \dot{m}_{\text{FEEDBK}} + \dot{m}_{\text{FLOWIN}}) + (1 - \phi) \dot{P}_{\text{OXY},\text{FLOWIN}} \quad (63)$$

If  $1 < \phi$ :

$$m_U dc_{\text{FUEL},U}/dt = -c_{\text{FUEL},U} (\dot{m}_{\text{FEEDBK}}/\phi + \dot{m}_{\text{FLOWIN}}) + (1 - 1/\phi) \dot{P}_{\text{FUEL},\text{FLOWIN}} \quad (64)$$

$$m_U dc_{\text{OXY},U}/dt = -c_{\text{OXY},U} (\dot{m}_{\text{FEEDBK}} + \dot{m}_{\text{FLOWIN}}) \quad (65)$$

subject again to the initial conditions of Eqs. (54).

According to the assumptions at the beginning of this section,  $\dot{P}_{\text{FUEL},\text{FLOWIN}}$  and  $\dot{P}_{\text{OXY},\text{FLOWIN}}$  are specified for a given experimental run. Also specified would be the value of r for the fuel being used, e.g., as with the value for methane given in Eq. (34). Then  $\phi^{(\text{SS})}$  can be calculated from Eq. (19), and, from Eqs. (40), (45), and (47), the value of  $\dot{m}_{\text{FEEDBK}}$  is

$$\dot{m}_{\text{FEEDBK}} = \begin{cases} (c_{\text{FUEL},U}/c_{\text{FUEL},U}^{(\text{MAX})})(1 - \phi^{(\text{SS})}) \cdot \text{OXY, FLOWIN } r/c_{\text{FUEL},U}^{(\text{MAX})} & \text{if } 0 \leq \phi^{(\text{SS})} \leq 1 \\ (c_{\text{OXY},U}/c_{\text{OXY},U}^{(\text{MAX})})(1 - 1/\phi^{(\text{SS})}) \cdot \dot{P}_{\text{FUEL},\text{FLOWIN}}/(c_{\text{OXY},U}^{(\text{MAX})} r) & \text{if } 1 < \phi^{(\text{SS})} \end{cases} \quad (66)$$

Solutions for the two ranges of  $\phi^{(\text{SS})}$  will be obtained sequentially. Before discussing these, it is noted from Eqs. (19) and (51) and from the first initial condition of Eq. (54) that  $\phi(t=0)$  will always satisfy

$$\phi(t=0) \leq \phi^{(\text{SS})} \quad (67)$$

As t increases from zero,  $\phi(t)$  will be expected to increase monotonically with t between  $\phi(t=0)$  and  $\phi^{(\text{SS})}$ .

Case 1:  $0 \leq \phi^{(\text{SS})} \leq 1$

Here the top portion of Eq. (66) provides the required value for  $\dot{m}_{\text{FEEDBK}}$ . Using this in Eqs. (62) and (63) leads to

$$m_U dc_{\text{FUEL},U}/dt = -c_{\text{FUEL},U} \{ (c_{\text{FUEL},U}/c_{\text{FUEL},U}^{(\text{MAX})})(1 - \phi^{(\text{SS})}) \cdot \dot{P}_{\text{OXY},\text{FLOWIN}} r/c_{\text{FUEL},U}^{(\text{MAX})} + \dot{m}_{\text{FLOWIN}} \} \quad (68)$$

$$m_U dc_{\text{OXY},U}/dt = -c_{\text{OXY},U} \{ (c_{\text{FUEL},U}/c_{\text{FUEL},U}^{(\text{MAX})}) \phi (1 - \phi^{(\text{SS})}) \cdot \dot{P}_{\text{OXY},\text{FLOWIN}} r/c_{\text{FUEL},U}^{(\text{MAX})} + \dot{m}_{\text{FLOWIN}} \} + (1 - \phi) \dot{P}_{\text{OXY},\text{FLOWIN}} \quad (69)$$

Since  $c_{\text{FUEL},U}(t=0) = 0$ , it is evident from Eq. (68)

that  $dc_{FUEL,U}/dt$  is initially zero and will remain zero for all  $t$ . Therefore, for all  $t$

$$c_{FUEL,U}(t) = 0 \quad (70)$$

In view of Eqs. (70) and (66), for the assumed complete stoichiometric reaction the model predicts  $\dot{m}_{FEEDBK} = 0$  throughout an entire Case-1 experiment. Note that this is consistent with earlier discussion of  $\dot{m}_{FEEDBK}$  equations when  $c_{OXY,U} \geq 0$ ,  $c_{FUEL,U} = 0$ . Also, it is clear from Eqs. (19) and (51) that the  $\dot{m}_{FEEDBK} = 0$  result leads to the further conclusion that

$$\phi(t) - \phi(t=0) = \phi(ss) \quad (71)$$

The results of Eqs. (61), (70), and (71) lead to significant simplification of Eqs. (56) and (68) which become

$$m_U dc_{OXY,U}/dt = -c_{OXY,U} \dot{m}_{FLOWIN} + (1 - \phi(ss)) \dot{P}_{OXY, FLOWIN} \quad (72)$$

$$m_U dc_{k,U}/dt + c_{k,U} \dot{m}_{FLOWIN} = \dot{P}_{FUEL, FLOWIN} C_k \quad k \text{ not fuel or oxygen} \quad (73)$$

where, from Eqs. (60) and (61),  $C_{CO_2} = 11/4$  and  $C_{H_2O} = 9/4$  for  $CH_4$ .

It is convenient to define the characteristic time,  $t^*$ , dimensionless variables,  $\tau$ ,  $\psi_{OXY}$ ,  $\psi_k$ , and  $\mu$ , and the dimensionless parameter  $\beta$ :

$$\tau = t \dot{m}_{FLOWIN} / m_U(t=0) \quad (74)$$

$$- t \dot{m}_{FLOWIN} RT_U(t=0) / (V P_{AMB}) = \tau / t^* \quad (74)$$

$$\psi_{OXY} = c_{OXY,U}(t) / c_{OXY,U}(t=0) = c_{OXY,U}(t) / c_{OXY,U}^{(MAX)} \quad (75)$$

$$\psi_k = c_{k,U}(t) \dot{m}_{FLOWIN} / [\dot{P}_{FUEL, FLOWIN} f_k(\phi(ss))] \quad (76)$$

$k \text{ not fuel or oxygen}$

$$\mu = \mu(\tau) = m_U(t) / m_U(t=0) = T_U(t=0) / T_U(t) = T_U(t=0) / T_U(t^* \tau) \quad (77)$$

$$\beta = [(\phi(ss) - 1) \dot{P}_{OXY, FLOWIN} / \dot{m}_{FLOWIN}] / c_{OXY,U}^{(MAX)} - (1 - 1/\phi(ss)) / (c_{OXY,U}^{(MAX)} \tau + 1/\phi(ss)) \quad (78)$$

According to Eq. (27), for the present range of  $\phi(ss)$

$$\beta = - c_{OXY, REACTOUT, STOICH}^{(SS)} / c_{OXY,U}^{(MAX)} \quad (79)$$

if  $0 \leq \phi(ss) \leq 1$

Note that here  $\beta$  must satisfy

$$-1 \leq \beta \leq 0 \quad (80)$$

where  $\beta \rightarrow -1$  corresponds to  $\phi(ss) \rightarrow 0$  ( $\dot{P}_{FUEL, FLOWIN}$  becomes negligible and  $\dot{P}_{OXY, FLOWIN} / \dot{m}_{FLOWIN} \rightarrow c_{OXY,U}^{(MAX)} = 0.232$ ) and  $\beta = 0$  corresponds to  $\phi(ss) = 1$ , the upper limit for  $\phi(ss)$  in the present case.

Using Eqs. (74)-(78) in Eqs. (69) and (54) and in Eqs. (56) and (59), and making the final transformation

$$\sigma = \int_0^\tau d\eta / \mu(\eta) \quad (81)$$

leads to

$$d\psi_{OXY}/d\sigma = -\psi_{OXY} - \beta; \quad \psi_{OXY}(0) = 1 \quad (82)$$

$$d\psi_k/d\sigma = -\psi_k + 1; \quad \psi_k(0) = 0 \quad (83)$$

for  $k$  other than fuel or oxygen

The solutions to Eqs. (82) and (83) are

$$(\psi_{OXY} + \beta)/(1 + \beta) = \exp(-\sigma) \quad (84)$$

$$\psi_k = 1 - \exp(-\sigma) \quad k \text{ not fuel or oxygen} \quad (85)$$

The solution concentrations  $c_{OXY,U}(t)$  and  $c_{k,U}(t)$  of Eqs. (84) and (85) exhibit the expected transition from their initial to their steady state values, the latter corresponding to  $\lim \sigma \rightarrow \infty$  ( $\psi_{OXY}, \psi_k = (-\beta, 0)$ ). Here the transition process involves simple dilution of the upper layer by the steady and constant stream (i.e., corresponding to  $\phi = \phi(ss) = \text{constant}$ ) flowing from the reactor. Plots of these results will be presented below.

Case 2:  $1 < \phi(ss)$

Here the bottom portion of Eq. (66) provides the value for  $\dot{m}_{FEEDBK}$ , which is no longer zero. Using this in Eq. (51) along with the initial conditions of Eqs. (54), it can be shown that for all possible experimental runs covered by the present Case 2, the model predicts  $\phi(t=0) = 1$ . Accordingly, from Eqs. (62)-(65), only Eqs. (64) and (65) need to be considered.

The dimensionless variable  $\psi_{FUEL}$  is defined as

$$\psi_{FUEL} = c_{FUEL,U} / c_{FUEL, REACTOUT, STOICH}^{(SS)} \quad (86)$$

Also, from Eq. (26), for the present range of  $\phi(ss)$

$$\beta = c_{FUEL, REACTOUT, STOICH}^{(SS)} / (c_{OXY,U}^{(MAX)} \tau) \quad \text{if } 1 < \phi(ss) \quad (87)$$

Note that here  $\beta$  must satisfy

$$0 < \beta \leq 1 / (c_{OXY,U}^{(MAX)} \tau) \quad \text{if } 1 < \phi(ss) \quad (88)$$

According to Eq. (78),  $\beta \rightarrow 1 / [c_{OXY,U}^{(MAX)} (\dot{P}_{FUEL} / \dot{P}_{OXY})_{STOICH}]$  corresponds to  $\phi(ss) \rightarrow \infty$ , i.e., an experiment with the fuel source embedded in the upper layer and with no oxygen supply ( $\dot{P}_{OXY, FLOWIN} = 0$ ), and  $\beta \rightarrow 0$  corresponds to  $\phi(t=0) = \phi(ss) \rightarrow 1$ . For  $CH_4$ , the upper limit for  $\beta \approx 1 / [0.232(1/4)] \approx 17.24$ .

Using Eqs. (19), (61), and (66) and the above definitions for  $\psi_{FUEL}$ ,  $\psi_{OXY}$ , and  $\beta$  in Eqs. (51), (57), (60), and (65) leads to

$$\text{If } 1 < \phi = \phi(ss) [1 + \beta(1 - 1/\phi(ss)) \psi_{FUEL} \psi_{OXY}] / [1 + (\phi(ss) - 1) \psi_{OXY}^2] \quad (89)$$

$$d\psi_{FUEL}/d\sigma = \quad (90)$$

$$- (\beta \psi_{OXY} + 1) \psi_{FUEL} + [1 + \beta \psi_{OXY} \psi_{FUEL} - \psi_{OXY}^2] / [1 + \beta(1 - 1/\phi(ss)) \psi_{OXY} \psi_{FUEL}]$$

$$d\psi_{OXY}/d\sigma = - (\beta \psi_{OXY} + 1) \psi_{OXY} \quad (91)$$

$$d\psi_k/d\sigma + \psi_k = [\psi_{OXY}^2 (1 - 1/\phi(ss)) + 1/\phi(ss)] \quad (92)$$

$k \text{ not fuel or oxygen}$

$$\psi_{\text{OXY}}(0) = 1; \psi_{\text{FUEL}}(0) = 0; \quad (93)$$

$$\psi_k(0) = 0 \text{ k not fuel or oxygen}$$

Note that in obtaining Eq. (92), the second of Eqs. (61) was used to show that for complete stoichiometric combustion and for any  $\phi > 1$ , as is the case here,

$$\phi f_k(\phi) / [\phi^{(SS)} f_k(\phi^{(SS)})] = 1 \text{ for all k} \quad (94)$$

The solution of Eqs. (91) and (93) for  $\psi_{\text{OXY}}$  is found to be

$$\psi_{\text{OXY}} = \exp(-\sigma) / (1 + \beta [1 - \exp(-\sigma)]) \quad (95)$$

and this is plotted in Figure 9 with parameter  $\beta$  in the range  $0 < \beta \leq 20$ . Using Eq. (95), the solution of Eqs. (92) and (94) for  $\psi_k$  is found to be

$$\psi_k = [1 - \exp(-\sigma)] [1/\phi^{(SS)} + (1 - 1/\phi^{(SS)})\psi_{\text{OXY}}] \quad (96)$$

Eq. (95) was used to numerically integrate Eqs. (90) and (93) for  $\psi_{\text{FUEL}}$ .

**Plots and discussion of the solutions.** The solutions for  $\psi_{\text{OXY}}$ ,  $\psi_{\text{FUEL}}$ , and  $\psi_k$  are plotted in Figures 9 and 10 for the entire range of  $\beta$  and  $\phi^{(SS)}$ , respectively. To prepare these plots it was convenient to use the following result obtained from Eq. (78)

$$\phi^{(SS)} = (1 + \beta) / (1 - \beta c_{\text{OXY},0}^{\text{MAX}} r) \quad (97)$$

The Figure 9 plots present the dimensionless concentrations as a function of dimensionless time with  $\beta$  as a parameter.

Consistent with the Case-1 results of Eqs. (84) and (85), in the entire range  $-1 \leq \beta \leq 0$   $\psi_k$  is seen in Figure 9 to be independent of both  $\beta$  and fuel-type, i.e.,  $r$ , while  $\psi_{\text{OXY}}$  depends on  $\beta$ , but is otherwise independent of fuel-type. Also, for this  $\beta$  range and for the corresponding  $\phi^{(SS)}$  range  $0 \leq \phi^{(SS)} \leq 1$ , fuel concentration is identically zero according to Eq. (70) and no dimensionless variable for this concentration was required in the analysis.

Consistent with the Case-2 results of Eqs. (90), (93), (95), and (96) and by the definition of Eq. (78), for  $\beta > 0$  all dimensionless concentrations depend on both  $\beta$  and fuel-type except for that of oxygen which only depends on  $\beta$ . In this range of  $\beta$ , the actual results plotted in Figure 9 are those that correspond to the use of  $\text{CH}_4$  as the fuel, i.e.,  $r$  taken to be  $1/4$ .

Recall that  $\beta > 0$  is a necessary condition for the steady state value of  $c_{\text{FUEL},U}$  to be non-zero, and that  $\psi_{\text{FUEL}}$  was defined only in this  $\beta$  range as the concentration  $c_{\text{FUEL},U}$  made dimensionless by normalizing with its steady state value. Thus, as indicated in the plots,  $\psi_{\text{FUEL}}$  solutions only exist for  $\beta > 0$ . It is noteworthy that for  $\text{CH}_4$ ,  $\psi_{\text{FUEL}}$  is relatively insensitive to variations in  $\beta$  in the entire applicable range of  $\beta$ .

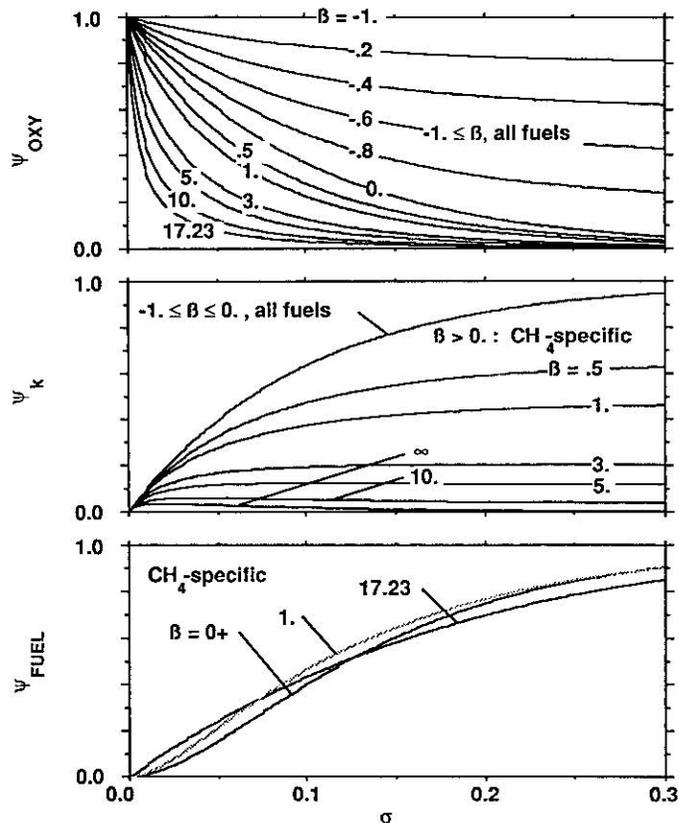


Fig. 9. Plots of dimensionless concentrations  $\psi_{\text{OXY}}$ ,  $\psi_k$ , and  $\psi_{\text{FUEL}}$  as a functions of dimensionless time,  $\sigma$ , with  $\beta$  as a parameter, where the results, are fuel-independent for  $-1 \leq \beta \leq 0$ , and  $\text{CH}_4$ -specific for  $\beta > 1$ .

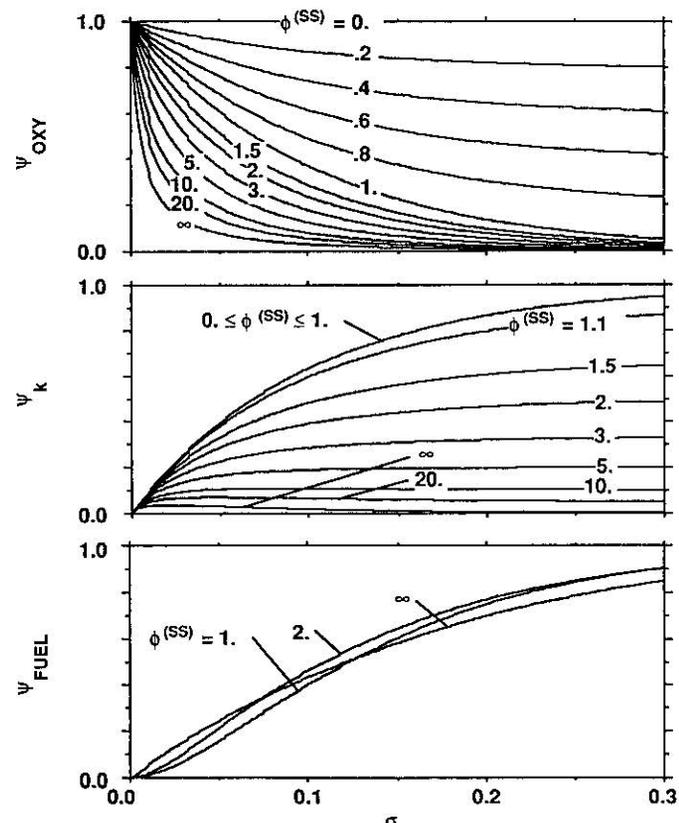


Fig. 10. Plots of dimensionless concentrations  $\psi_{\text{OXY}}$ ,  $\psi_k$ , and  $\psi_{\text{FUEL}}$  as a functions of dimensionless time,  $\sigma$ , with  $\phi^{(SS)}$  as a parameter when  $\text{CH}_4$  is the fuel, i.e., when  $(P_{\text{FUEL}}/P_{\text{OXY}})_{\text{STOICH}} = 1/4$ .

All results are also presented in Figure 10, where plots of the  $\psi$ 's are given as functions of  $\sigma$  with  $\phi^{(ss)}$  as a parameter. Such plots depend on fuel-type for the entire range of  $\phi^{(ss)}$ . The actual plots presented correspond again to use of  $\text{CH}_4$  as the fuel.

Figure 11 highlights the  $\psi$  solutions when  $\phi^{(ss)} \rightarrow \infty$  and when  $\text{CH}_4$  is the fuel, i.e., when  $\beta \approx 17.23$ . As mentioned earlier, this corresponds to experimental runs where the fuel is methane and where the fuel source is submerged in the upper layer with no source of oxygen. As has been observed by Morehart and Zukoski (1988), such configurations lead to extinguishment of the flame at the time when  $c_{\text{OXY},U}$  drops to approximately 0.15, i.e., when  $\psi_{\text{OXY}}$  drops to  $0.15/0.23 = 0.65$ . As can be seen in the figure, this is predicted to occur when  $\sigma$  is approximately  $\sigma_{\text{EXT}} = 0.0030$ . Thus, using the complete stoichiometric combustion approximation, the present model predicts that a methane flame will extinguish in a Figure 4b experiment at the time,  $t_{\text{EXT}}$ , when

$$\int_0^{t_{\text{EXT}}} \left[ \frac{T(t)}{T(t=0)} \right] dt - t^* \sigma_{\text{EXT}} = 0.0030 V_{\text{PAMB}} / [m_{\text{FLOWIN}} RT_U(t=0)] \quad (98)$$

#### SUMMARY AND CONCLUSIONS

A general model was developed for predicting the generation rates of oxygen, fuel, and any other products of combustion of interest in rooms containing a fire. The model is called the Generalized Global Equivalency Ratio Model (GGERM). It extends the Steady State Global

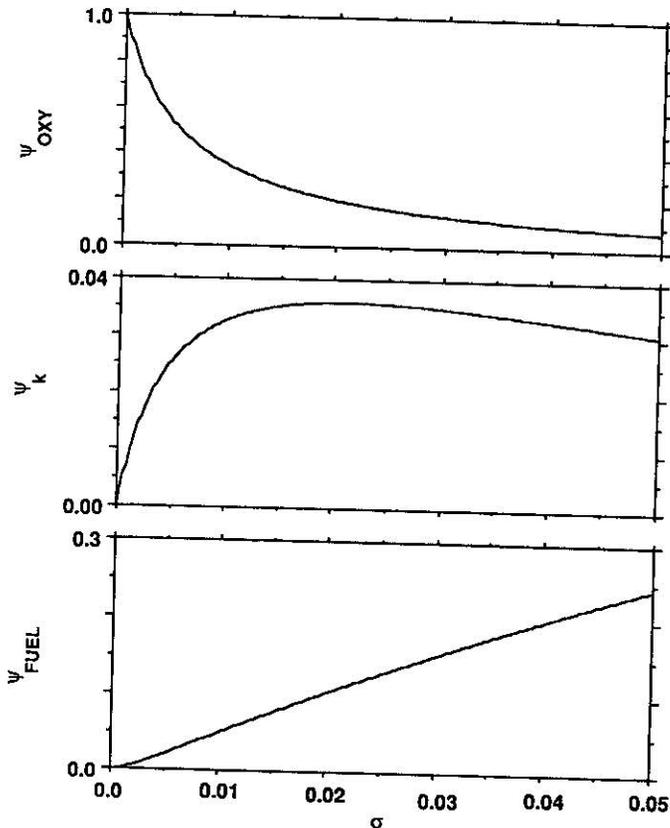


Fig. 11. Plots of dimensionless concentrations  $\psi_{\text{OXY}}$ ,  $\psi_k$ , and  $\psi_{\text{FUEL}}$  as a functions of dimensionless time,  $\sigma$ , when  $\phi^{(ss)} \rightarrow \infty$  and when  $\text{CH}_4$  is the fuel, i.e.,  $\beta \approx 17.23$ .

Equivalence Ratio Model (SSGERM) established previously in the steady-state experimental studies of Beyler (1986a, 1986b), Toner, Zukoski, and Kubota (1986), and Zukoski et al (1989, 1991).

A concise algorithm was presented for implementing the model in two-layer zone-type fire models. This would be used in simulating the distribution of products of combustion in multi-room fire environments.

The last section was devoted to an example application of the GGERM. There, the model was used to formulate the general initial-value problems for the transient concentrations of all products of combustion in some of the above-mentioned experimental studies. The problems were solved under the constraint that only complete stoichiometric combustion processes are involved. Solutions for the concentrations were obtained and presented for arbitrary experimental conditions. As a final result, the solutions were used to predict the time-to-extinguishment of a burning fuel source embedded in an initially ambient-atmosphere upper layer.

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