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Transient Catalytic Combustor Model

James S. T'ien
Case Western Reserve University

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National Aeronautics and Space Administration
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ABSTRACT

A lean combustion model for monolithic catalytic combustors is given. The model, consisting of several semi-global chemical reaction steps in the gas phase and on the surface, is capable of analyzing CO and THC emissions and combustor efficiency in both steady and unsteady states.

In the steady-state model computation presented, the influence of operating and design parameters on the minimum combustor length is studied. Special attention is given to the effect of after-bed gas phase reaction space. Comparison with experimental data by Anderson indicates good agreement in the range of parameters covered.

In the transient analysis, a quasisteady gas phase and a thermally-thin substrate are assumed. The combustor response delay is due to the substrate thermal inertia. Fast response is found to be favored by thin substrate, short catalytic bed length, high combustor inlet and final temperatures and, in most cases, small gas channel diameters. The calculated gas and substrate temperature time history at different axial positions provide an understanding of how the catalytic combustor responds to an upstream condition change. The computed results also suggest that the gas residence times in the catalytic bed and in the after-bed space are correlatable with the nondimensional combustor response time. When fast transient responses are required, both steady and unsteady studies have to be made to achieve a meaningful compromising design.

INTRODUCTION

The operation and the design of catalytic combustors are limited on one end by the high temperature that the catalysts can tolerate and on the other end (low temperature) by the acceptable emission levels of CO and unburnt hydrocarbons. The aim of the combustion engineer is to design a compact and durable combustor capable of efficient and clean combustion. Catalytic combustor modeling can contribute to this objective by providing more understanding to the detail processes occurring in the reactor and to serve as a design guidance for minimizing the numbers of experimental tests needed.

There are several steady-state catalytic combustor models in existence (Ablow and Wise, 1979, Cerkanowicz, et al, 1977,Kelley et al, 1977, Kendall et al, 1979) and they show a high degree of success in describing the events occurring in the combustor. In particular, the model by Kelley et at (1977) containing detailed gas phase chemistry for methane/air reactions can predict pollutant emissions. Detailed kinetics, unfortunately, are not yet available for most other practical fuels. Since emission characteristics are important considerations for catalytic combustor design, in the absence of more detailed information, models consisting of several key semi-global chemical steps seem appropriate.

In addition to the emission characteristics, the transient behavior of catalytic combustors is expected to be different from that of a conventional gas turbine burner, due to the large thermal inertia of the substrate. Non-steady operations are obviously important to transportation engines since their power levels have to be changed frequently. Transients may also be a concern with stationary gas turbine applications, since the

ignition/shutdown operation can produce excessive thermal stress or thermal shock if the combustor is not designed or operated properly and the substrate can fail as a result (DeCorso and Carl, 1979).

Typical questions concerning transient operations include the combustor response time, the type of response, the unsteady substrate temperature history and the resultant thermal stress distribution. At the present time, both experiment and theory on transient catalytic combustion are lacking. A model is presented here attempting to analyze the problem theoretically. In Chapter I of this report, the transient combustion model will be formulated and numerical solution will be presented as a parametric study. Since the transient computer code can also yield steady-state results, in Chapter II, a detailed computation of steady states is given and a comparison with Anderson's data is made. As far as the combustion models are concerned, the one in Chapter II has a three-step global gas-phase chemical reaction vs. a two-step one in Chapter II. The reason for using the three-step scheme is discussed in the beginning of Chapter II.

CHAPTER I TRANSIENT CATALYTIC COMBUSTOR MODEL

I.1 Nonsteady Combustion Model

Consideration of Time Scales

For a monolithic catalytic combustor with uniform cell distribution in the plane normal to the approaching flow direction, if the combustor wall is well insulated, then the study of the whole reactor can be reduced to the consideration of a single cell unit. Referring to Fig. I.1, each cell unit consists of an open gas channel, the associated substrate volume and an after-bed gas reaction space.

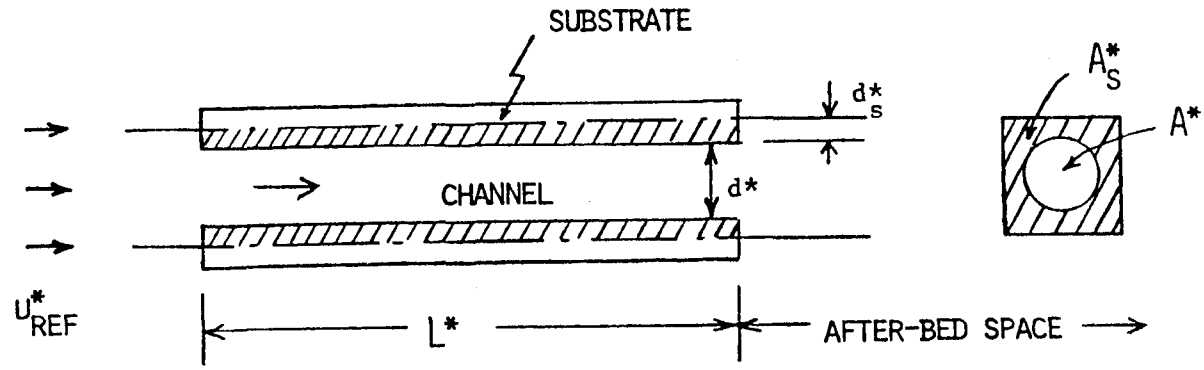

Figure I.1 Schematic Drawing of One Cell Unit

Considering first the steady-state combustion, the relevant time scales are the gas residence time in the reactor, the heat and mass transfer time between the gas and the solid surface inside the channel and the gas-phase and surface reaction times. When a transient is caused by an upstream parameter variation, then the new time scales involved include the input characteristic time, the time for the temperature wave to reach the central plane of the substrate and the time for heating-up (or cooling-down) the substrate.

Table I defines these characteristic times and their estimated magnitudes. It should be noted that some of the time scales vary along the channel of the reactor bed. For example, the heat/mass transfer time and the substrate heat-up time are shorter at the flow entrance region than those for far downstream, and the ones used in Table I are those based on fully-developed flow profiles. However, the estimation from Table I does serve the purpose of order-of-magnitude comparison. From this table we see that the longest time is the solid heat-up time, being of the order of seconds. If the time scale we are interested in is much greater than the gas residence time (~15 msec), then the gas phase processes (including heat/mass transfer and chemical reactions) can be regarded as in a quasi-steady state. If furthermore the substrate half-thickness is smaller than about .2 mm, then the substrate temperature distribution in the direction normal to the channel axis can be regarded as uniform at any given time. In this limiting case then, a "quasi-steady-gas-phase and thermally-thin-substrate" model is applicable with the only transient process being the substrate heating-up or cooling-down. In the following section, this model will be described in mathematical form.

Quasisteady Gas Phase

Quasisteady gas phase implies that the differential equations for the

Table I.1 Estimate of Transient Time Scales in Catalytic Monolith Combustor

Time	Definition	Estimated Magnitude
Gas residence time in reactor bed	$(L^*/u^*_{ref})\,(A^*/A^*_T)$	1 - 15 msec
Gas residence time in after-bed space	L^*_{as}/u^*_{ref}	0 - 15 msec
Heat/mass transfer time between gas and solid surface in channel	$\frac{1}{Nu_\infty}\,\frac{1}{\pi}\,\frac{d^{*2}}{4\alpha^*(0,0)}$	.5 - 7.5 msec for $d^* \leq 3.6$ mm
Chemical reaction times (gas-phase and heterogeneous)		Same order of magnitude as gas residence times
Time for temperature wave to reach the substrate center plane	$\frac{d^{*2}_s}{\alpha^*_s}$	0.5 - 25 msec for $d^*_s \leq .2$ mm
Substrate heat-up time	$\frac{1}{Nu_\infty}\,\frac{1}{\pi}\,\frac{A^*_s \rho^*_s C^*_s}{k^*(0,0)}$	0.5 sec - 20 sec
Transient input time		variable, specified

gas-phase processes are the same as those for the steady state. Only the boundary conditions on the solid surface are different. There are several steady-state catalytic combustor models in existence [Cerkanowicz et al, 1977, Kelly et al, 1977, 1979] and they show a high degree of success in describing the events occurring in the combustor. In particular, the model by Kelley et al (1977) containing detailed chemistry for methane/air reactions can predict pollutant emissions. Detailed kinetics, unfortunately, are not yet available for most other practical fuels. Since emission characteristics are important considerations for catalytic combustor design, in the absence of more detailed information, a model consisting of several key semi-global chemical steps is proposed.

For fuel-lean catalytic combustion using nitrogen-free hydrocarbon fuels, the NO_x emission is negligible because of low flame temperatures. The only pollutants needed to be considered are unburnt hydrocarbons (UHC) and carbon monoxide (CO). For this reason, the two semi-global chemical reactions used in the gas phase are:

(A) $$C_nH_m + 1/2\ (n + m/2)\ O_2 \rightarrow n\ CO + m/2\ H_2O$$

$$\frac{d[C_nH_m]}{d\ t^*} = -\ C_1^*\ p^{*\alpha_1}\ [C_nH_m]^{\alpha_2}[O_2]^{\alpha_3}\ T^{*\alpha_4}\ \exp\ (-E_1^*/RT^*) \qquad (1)$$

(B) $$CO + 1/2\ O_2 \rightarrow CO_2$$

$$\frac{d[CO]}{d\ t^*} = -C_2^*\ p^{*\beta_1}\ [CO]^{\beta_2}[O_2]^{\beta_3}[H_2O]^{\beta_5}\ T^{*\beta_4}\ \exp\ (-E_2^*/RT^*) \qquad (2)$$

In describing the flow in the reactor channel, we follow previous investigators in using the plug flow approximation. For transient cases, in general, the fluid properties are functions of x, the distance along the channel axis and t, the time. For example, density of the gas will be

expressed as $\rho(x,t)$. The nondimensional forms of these equations are summarized in the following (supscript * denotes dimensional quantity and without * denotes nondimensional quantities).

Continuity: $\rho u = \hat{\rho}(o,t)\ u(o,t)$ (3)

Momentum: $p = p(o,t)$ (4)

Energy:
$$\rho u \frac{\partial T}{\partial x} + J_H(T - T_s) = q_1 Y_{HC}(0,0)\ w_1 + q_2 Y_{HC}(0,0)\ w_2 \quad (5)$$

Species:

Hydrocarbon:
$$\rho u \frac{\partial \mathcal{Y}_{HC}}{\partial x} + J_{D_1}(\mathcal{Y}_{HC} - \mathcal{Y}_{HC,S}) = - w_1 \quad (6)$$

Carbon monoxide:
$$\rho u \frac{\partial \mathcal{Y}_{CO}}{\partial x} + J_{D_2}(\mathcal{Y}_{CO} - \mathcal{Y}_{CO,S}) = w_1 C_n - w_2 \quad (7)$$

Oxygen:
$$\mathcal{Y}_{O_2} = 1 - \phi(1 - \mathcal{Y}_{HC}) + \frac{1}{2}\ \mathcal{Y}_{CO}\ \left(\frac{Y_{HC}(0,0)}{Y_{O_2}(0,0)} \frac{W_{O_2}}{W_{CO}} \right) \quad (8)$$

Equation of state: $p = \rho T$ (9)

The reaction rates are given by
$$w_1 = B_1\ p^{\alpha_1}\ \rho^{(\alpha_2 + \alpha_3)} T^{\alpha_4}\ \mathcal{Y}_{HC}^{\alpha_2}\ \mathcal{Y}_{O_2}^{\alpha_3}\ e^{-(E_1/T)} \quad (10)$$

$$w_2 = B_2\ p^{\beta_1}\ \rho^{(\beta_2+\beta_3+\beta_5)} T^{\beta_4}\ \mathcal{Y}_{CO}^{\beta_2}\ \mathcal{Y}_{O_2}^{\beta_3}\ Y_{H_2O}^{\beta_5}\ e^{-(E_2/T)} \quad (11)$$

and
$$Y_{H_2O}(x,t) = \frac{m}{2} \frac{W_{H_2O}}{W_{HC}}\ Y_{HC}^{(0,0)} \left[\mathcal{Y}_{HC}(o,t) - \mathcal{Y}_{HC}(x,t) \right] \quad (12)$$

The definition of B_1 and B_2 can be found in the nomenclature.

In deriving Eqns (5-8), heat conduction and mass diffusion in the axial direction are neglected because the Peclet number based on typical gas velocity (>10 M/sec) is much greater than unity [Ablow and Wise, 1979]. The dimensionless lateral heat and mass transfer coefficients J_H and J_{Di}, in Eqns (5-7) are derived from Nusselt number calculation in entrance flow in a tube of constant surface temperature [Kays, 1966]. Following Kelly et al (1977), a modification is made at the entrance point based on local stagnation flow estimation. The use of entrance flow transport properties, rather than fully-developed constant values, make a great difference in the temperature and species distributions in the flow entrance region.

The above system of equations can also be applied to the after-bed space where only gas-phase reactions occur. This is done by putting J_H and J_{Di} equal to zero in Eqns (5-7) and by properly changing the mass flux per unit area in Eq (3) due to area change.

Unsteady Solid with Thin-Wall Substrate

When the substrate wall is thermally thin, the solid temperature can be regarded as a function of axial distance and time only, i.e., $T_s(x,t)$. The energy balance of the solid, including the solid surface, results in the following equation:

$$A_s^* \rho_s^* C_s^* \frac{\partial T_s^*}{\partial t^*} - h_T^* S^* (T^* - T_s^*) = S^* [q_3^* J_3^* + q_4^* J_4^*] \qquad (13)$$

In Eq (13) the heat conduction in the axial direction in the solid is neglected in comparison with the heat transfer rate between the gas and solid across the gas channel.

Two semi-global catalytic surface reactions are assumed. They are

$$(C) \quad C_nH_m + (n + \frac{m}{4})\, O_2 \rightarrow nCO_2 + \frac{m}{2}\, H_2O \tag{14}$$

with the corresponding surface reaction rate J_3^* given by

$$J_3^* = C_3^* [C_nH_m]_s \; e^{-E_3^*/RT_s^*}$$

$$\text{and} \quad (D) \quad CO + \frac{1}{2}\, O_2 \rightarrow CO_2 \tag{15}$$

$$\text{with} \qquad J_4^* = C_4^* [CO]_s \; e^{-E_4^*/RT_s^*}$$

In surface reaction (C), the hydrocarbon is oxidized to form CO_2 and H_2O, not CO such as in gas-phase reaction (A). This is based on the present available experimental evidence in oxygen-rich systems, only CO_2, not CO, is found on or close to the catalytic surface [Schwartz et al, 1971, Anderson, 1976 and Marteney, 1979].

Eq (13) is non dimensionalized by first defining a proper reference time scale τ^*.

$$\tau^* \equiv \frac{1}{Nu_\infty}\, \frac{1}{\pi}\, \frac{A_s^*\, \rho_s^*\, C_s^*}{k^*(0,0)} \tag{16}$$

$$\text{and} \qquad t \equiv t^*/\tau^*$$

$$r_{nk} \equiv \frac{Nu_x}{Nu_\infty}\, \frac{k^*}{k^*(0,0)} \tag{17}$$

Eq (13) becomes

$$\frac{\partial T_s}{\partial t} - r_{nk}\,(T - T_s) = B_3 Y_{HC}(0,0)\; q_3 \rho\; \mathcal{Y}_{HC,s}\; \exp(-E_3/T_s)$$

$$+ B_4 Y_{HC}(0,0) q_4 \rho\; \mathcal{Y}_{CO,s}\; \exp(-E_4/T_s) \tag{18}$$

Neglecting transient accumulation on the surface, the surface hydrocarbon and carbon monoxide are given by

$$r_{nk}\left(\gamma_{HC} - \gamma_{HC,s}\right) = \frac{1}{(L_{e_1})^{2/3}} B_3 \rho \gamma_{HC,s} \exp(-E_3/T_s) \quad (19)$$

$$r_{nk}\left(\gamma_{CO} - \gamma_{CO,s}\right) = \frac{1}{(L_{e_2})^{2/3}} B_4 \rho \gamma_{CO,s} \exp(-E_4/T_s) \quad (20)$$

Initial and Boundary Conditions

The system of equations (3-12, 18-20) needs initial and boundary conditions. Initial conditions (at t = 0) are required for T_s, $(\gamma_{HC})_s$ $(\gamma_{CO})_s$ as a function of x and upstream boundary conditions (at x = 0) should be specified for γ_{HC}, γ_{CO}, γ_{O2}, T, p and u as a function of time. These conditions depend on the types of transient input which can vary with engine designs and mode of operations. In the present paper, a simple start-up transient is investigated, i.e. catalytic combustor response to a step-wise fuel injection.

The substrate temperature at time t=0 is specified. This temperature can be the result of external heating of the substrate, say, by a torch. The fuel and air are then supplied at upstream. The model is intended to describe the events from t=0 to the final steady state. Mathematically, the conditions used are

$$
\begin{aligned}
T_s(x,0) &= \text{specified} \\
\mathcal{Y}_{HC,s}(x,0) &= 0 \\
\mathcal{Y}_{CO,s}(x,0) &= 0 \\
T(0,t) &= 1 \\
\mathcal{Y}_{HC}(0,t) &= 1 \\
\mathcal{Y}_{CO}(0,t) &= 0 \\
\mathcal{Y}_{O2}(0,t) &= 1 \\
p(0,t) &= 1 \\
u(0,t) &= 1
\end{aligned}
\qquad (21)
$$

Numerical Solution Procedure

Although most dependent variables in this problem are function of both x and t which, in general, results in partial differential equations, the assumption of quasisteady gas phase and thermally thin substrate greatly simplifies the mathematical property of the system and results in a simpler solution procedure.

The gas-phase differential equations (5-7) have only first derivative in x with t as a parameter, the solid equation (18) has only derivative in t with x as a parameter; therefore, they can be integrated at each time (t) or position (x) as ordinary differential equations using Runge-Kutta method. The procedure is started by first integrating Eqns (5-7) forward in x from upstream to the end of combustor for T, $\mathcal{Y}_{HC}$, $\mathcal{Y}_{CO}$ using the solid surface

quantities specified by the initial conditions, then Eq (18) is integrated for one time step (Δt) to find $T_s(x, \Delta t)$ and Eqns (19,20) are solved algebraically to find $\mathcal{Y}_{HC,s}(x, \Delta t)$ and $\mathcal{Y}_{CO,s}(x, \Delta t)$. These surface quantities are substituted back to Eqns (5-7) to start another cycle of integration. Steady-state and transient solutions are obtained using the same code. The computational time ranges from 10-50 seconds in a VAX-11 computer. The numerical scheme is an efficient one and it is suitable for parametric studies.

I.2 Computed Results

Steady State

Selected steady-state results will be presented first to facilitate the discussion on the transient response. Specifically, the relative importance of the catalytic bed length and the after-bed-gas-phase-reaction distance will be shown. In previous theoretical models, emphasis was placed on the combustion inside the catalytic bed only. The contribution of gas-phase reactions in the downstream space after the bed has been demonstrated in the experiments by T'ien and Anderson (1979) and Anderson (1980). Utilization of the pure gas-phase reactions in the downstream of the monolith to replace a portion of the catalytic bed will be shown to be crucial in reducing the catalytic combustor transient response time.

Table I.2 lists the values of chemical kinetic constants for reactions A to D used in this chapter. The hydrocarbon fuel chosen is propane. Semi-global kinetics for hydrocarbon and CO oxidation are from Edelman (1969) and Dryer and Glassman (1973) respectively, with the pre-exponential factors

Table I.2 Chemical Kinetic Constants for Chapter I

Reaction (A)	Reaction (B)	Reaction (C)	Reaction (D)
$C_1^* = 1.5 \times 10^5$	$C_2^* = 0.71 \times 10^{14}$	$C_3^* = 2.5 \times 10^3$	$C_4^* = 10^5$
$\alpha_1 = 0.3$	$\beta_1 = 0$	$E_3^* = 10$ (kcal/mole)	$E_4^* = 17.8$ (kcal/mole)
$\alpha_2 = 0.5$	$\beta_2 = 1$		
$\alpha_3 = 1$	$\beta_3 = 0.25$		
$\alpha_4 = 1$	$\beta_4 = 0$		
$E_1^* = 24$ (kcal/mole)	$\beta_5 = 0.5$		
	$E_2^* = 40$ (kcal/mole)		

adjusted. The activation energies for reactions C and D are obtained from the data of Marteney (1979) and Kuo and Morgan (1971) respectively with adjusted pre-exponential factors. It should be noted that the surface reaction rates contain information on catalyst type and loading density as well as the washcoat properties.

The design parameters considered are d*, channel hydraulic diameter, A^*/A_T^*, the percentage of open area (or equivalently, A^*/A_s^*, the ratio of open-to-close areas), L*, the catalytic bed length and L_{as}^*, after-bed gas-phase reaction length. The minimum catalytic combustor length required to reach the emission goal in steady-state operations is denoted using the subscript EG. The emission goal is chosen to be 1.64 g/kg of fuel for UHC and 13.6 g/kg of fuel for CO [Anderson, 1977]. The operating parameters include p*, the pressure, T_{in}^*, combustor inlet temperature, T_{af}^*, adiabatic flame temperature (or equivalently the fuel/air equivalence ratio ϕ) and U_{ref}^*, the reference velocity of the approach gas upstream of the reactor bed.

Fig. I.2 gives the profiles for one sample calculation. In this case, the propane fuel is oxidized quickly on the catalyst surface upon entering into the reactor channel and resulting in a high surface temperature, the gas temperature is raised by heat transfer from the substrate, gas-phase oxidation of propane is accelerated to form CO, and CO, in turn, is oxidized by both gas-phase and surface reactions to CO_2. Actually, two cases are shown in Fig.I.2. In one case, the reactor bed length is 4 cm, in the other, 8 cm. When the bed length is cut short at 4 cm, the surface oxidation reactions for the hydrocarbon fuel and CO stop there. This results in a higher CO concentration as shown by the dotted curve. The hydrocarbon curve

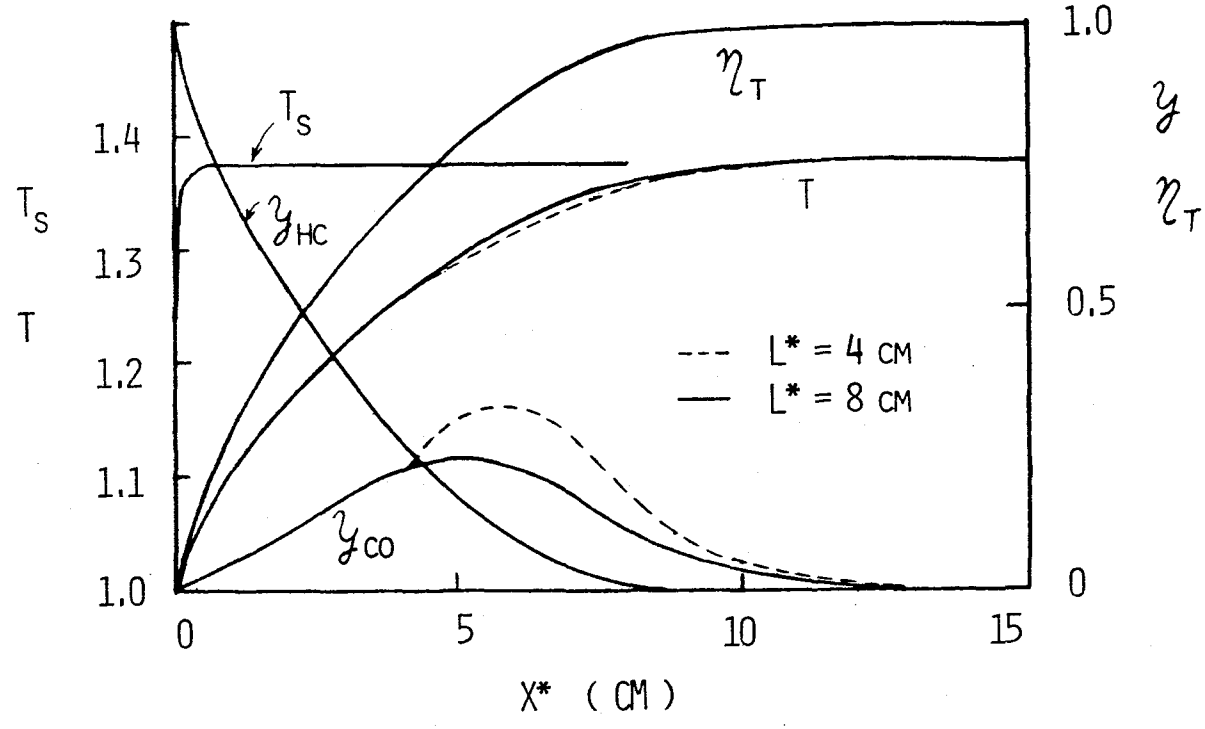

Figure I.2 Detailed steady-state profiles showing the effect of catalytic bed length. Operating conditions: $p^* = 3$ atm, $T^*_{in} = 1000°K$, $u^*_{ref} = 10$ m/s, $\phi = 0.15$, $d^* = 1.8$ mm and $A^*/A^*_T = .667$.

also shows a difference after 4 cm but the difference is too small to be shown clearly in this figure. The gas temperature is also lower in a portion of the combustor for the 4 cm case.

Fig. I.3 gives the combustor residence time required to reach the emission goal vs. the residence time in the catalytic bed. The "catalytic bed residence time", t_b^*, is defined by $L^*A^*/U^*_{ref}\ A^*_T$, where U^*_{ref} is the gas velocity upstream of the bed and the gas velocity inside the catalytic channel at the channel entrance is $U^*_{ref}A^*_T/A^*$, due to the area change. To be exact, the gas residence time in the bed should be $\int_o^{L^*} 1/U^* dx^*$ since the gas velocity in the channel, U^*, is changing continuously downstream due to the heat release. However, since $U^*(x)$ is not known until the solution is achieved, the catalytic bed residence time, t_b^*, as defined in Fig.I.3 is a good reference quantity and it is with this understanding when we use the terms of "bed residence time" and "combustor residence time".

Referring to the curve and the calculated points corresponding to T^*_{in} = 1000 K in Fig.I.3 we see that the residence times provide an excellent correlation for different values of U^*_{ref}, L^*, A^*/A^*_T and the required L^*_{as} to reach emission goals. As the catalytic bed residence time, t_b^*, increases, the total combustor residence time required to reach emission goals, t^*_{EG}, first decreases sharply and then levels off. The two other curves in Fig. I.3 give the effects of different combustor inlet temperatures. Higher inlet temperature required lower combustor residence time to reach emission goals for a fixed catalytic bed residence time. At 1200 K inlet temperature, no catalytic element is needed; emission goals can be reached in an acceptable gas residence time for a plug flow combustor without flame stabilizer (t_b^*= o and T^*_{EG} = 14 seconds). This has been verified by the recent

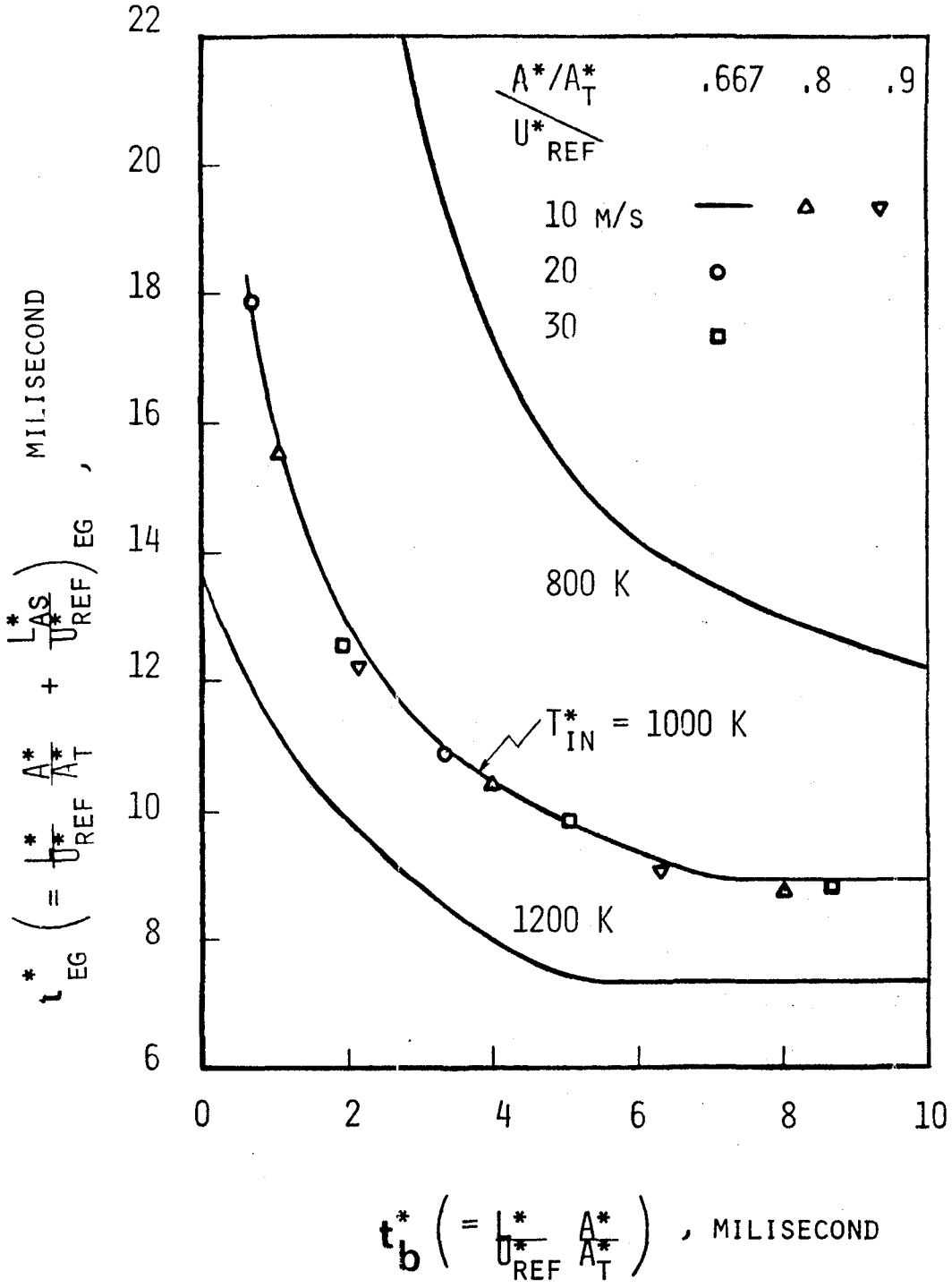

Fig. I.3 Minimum total combustor gas residence time for reaching emission goals (t^*_{EG}) vs. reactor bed residence time (t^*_b) as a function of combustor inlet temperature in steady-state operation. $p^* = 3$ atm, $d^* = 1.8$ mm and $T^*_{af} = 1370$ K.

experimental results of Anderson (1980b). Anderson's study also suggested the correlation using gas residence times (1980a).

Transient Response

One of the major concerns of the catalytic combustor application to transportation gas turbine engines is that the response time might be long. The computed transient results to be presented are combustor response to a stepwise increase of fuel flow rate (zero to a fixed value). Its purpose is to guide the search for "fast-response" catalytic combustor designs.

Some indication of the order of magnitude of the response time can be obtained from the definition of the characteristic time τ^* as defined in Eq (16). Small τ^* requires small thermal inertia, $A_s^* \rho_s^* C_s^*$. If the substrate density and heat capacity are fixed, small τ^* can be achieved with small solid crossectional area A_s^*, see Fig.I.1 for definition of A_s^*. It should be noted that there are other parameters such as catalytic bed length and channel diameter which will influence the response time and they are not contained in τ^*. This will be discussed later as we see the computed results.

The combustion efficiency at the end of the combustor will be used to characterize the combustor response time. There are two ways to define the combustion efficiency. One is the so-called "carbon-balanced" efficiency, η_{CB} [Anderson, 1975], where the combustion inefficiency is measured by the emission levels of CO and UHC and the energy carried away by them. The other efficiency is the ordinary one defined by the enthalpy rise across the combustor divided by the chemical energy available. If the gas specific heat is approximated as a constant, this efficiency, η_T, is given by $(T^* - T_{in}^*)/(T_{af}^* - T_{in}^*)$ where T^* is measured at the same location as the efficiency. For a perfectly insulated catalytic combustor in steady state,

η_{CB} and η_T are the same. However, the two are different in transient operations when there is a thermal lag in the substrate.

For the following transient calculation, the initial surface temperature condition is given by $T_s(x,0) = 1$, see Eq (21). For 1000°K inlet temperature, two bed lengths, 4 cm and 8 cm, are chosen for the transient calculation and efficiency is evaluated at their individual minimum combustor lengths according to Fig.I.3. Fig.I.4 shows the combustion efficiencies as a function of non-dimensional time. Looking at the curves for η_T (efficiency based on temperatures), the shorter bed (4 cm) combustor has a faster response than that of the longer bed (8 cm). If we take the time for η_T to reach 80% as an indication of characteristic response time, for the 4 cm bed, $t_{Ch} = 1.5$ and for the 8 cm bed, $t_{ch} = 2.5$; namely, the response time of 4 cm bed combustor is only 60% of that of the 8 cm bed combustor. From the consideration of steady-state operation alone, one would choose the 8 cm catalytic bed since, as can be deduced from Fig.I.3, this produces the shortest required combustor length (11 cm). However, combining transient and steady-state considerations, the 4 cm bed combustor may be a better choice as its response time is 60% of that of the 8 cm bed, with the total combustor length only slightly longer.

To understand why longer reactor bed results in a longer response time, surface and gas temperature distributions are plotted in Fig. I.5 as a function of time. From the substrate temperature distribution we see that during start-up transient, the solid temperature is higher in the flow entrance region as a result of higher mass transport and surface reaction rates. Comparing the solid and gas temperature histories for the case when catalytic bed length is 8 cm, we see that at t = 0.5, the solid is

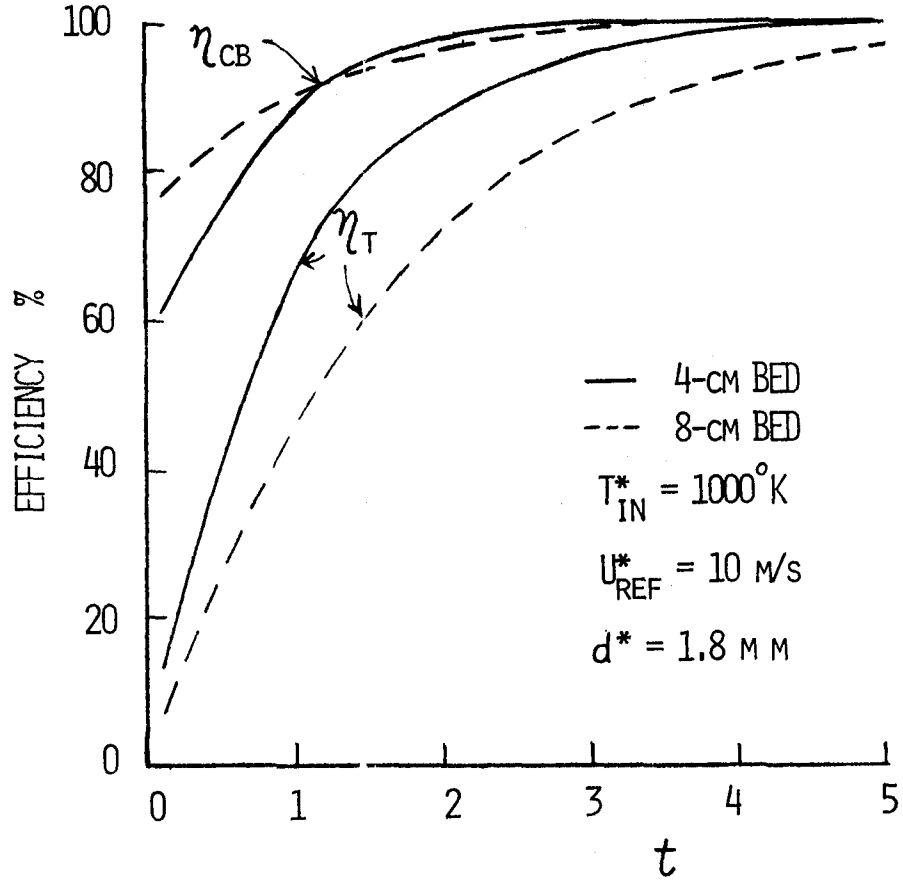

Fig. I.4 Combustion efficiencies as a function of time during start-up transient. $p^* = 3$ atm, $\phi = 0.15$ and $A^*/A^*_T = .667$.

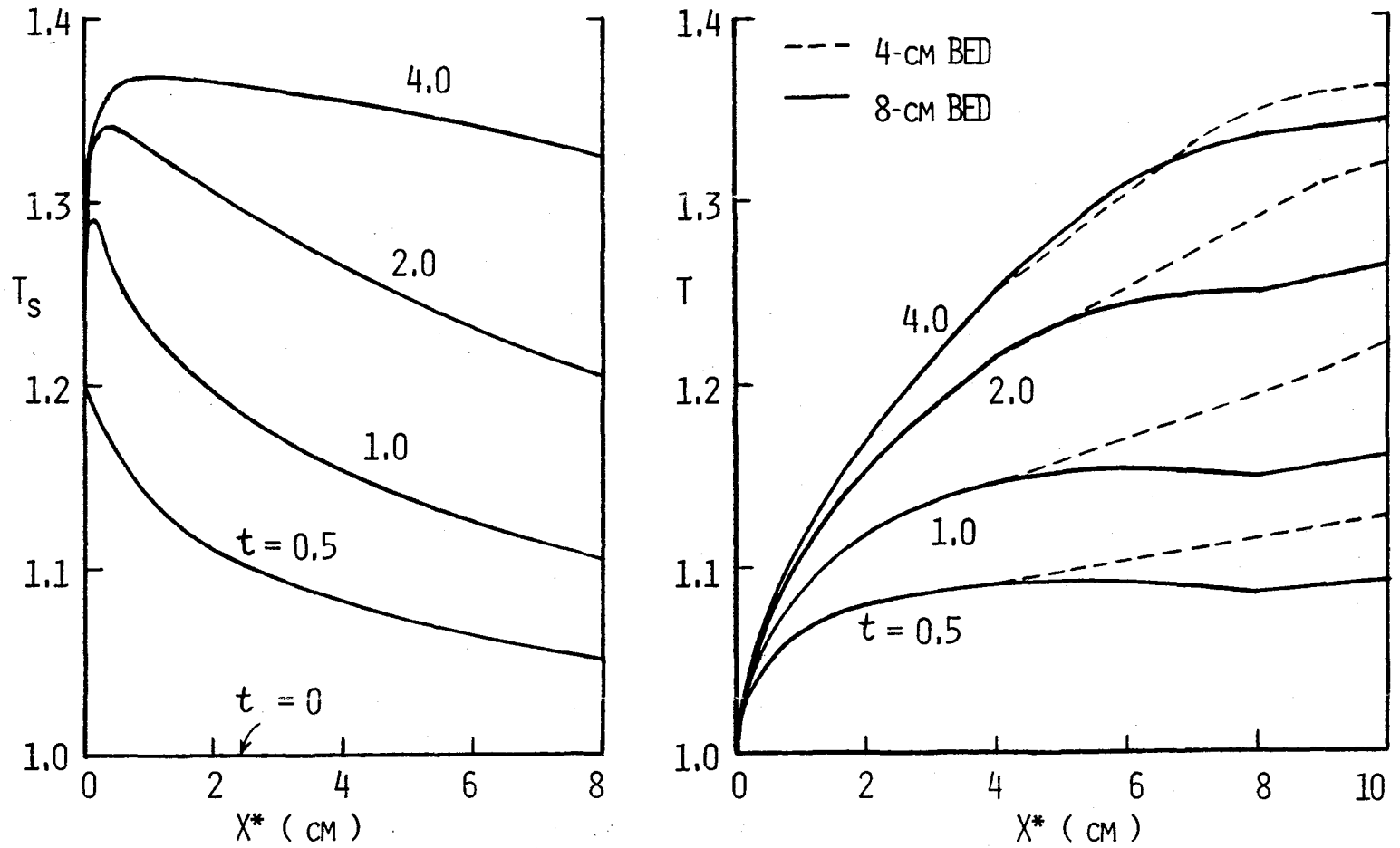

Fig.I.5 Gas and substrate temperature history during transient start-up for two bed lengths. Same operating and design parameters as those in Fig.I.4.

transfering heat to the gas in the upstream region in the bed. At $x^* = 3.5$ cm, the gas temperature becomes higher than the substrate temperature, heat is then transferred from the gas to the solid in the down-stream portion of the reactor channel. If the heat loss rate is greater than heat generation rate due to gas phase reactions, then the gas temperature will drop as shown in Fig.I.5. If we cut the reactor bed short at 4 cm, a portion of this heat loss can be eliminated and the downstream gas temperature ($x^* > 4$ cm) will be higher as indicated by the dotted curves in Fig.I.5. This explains why a shorter reactor bed can have a faster response.

More computation of the response time dependence on the catalytic bed length, gas velocity and combustor inlet temperature is shown in Fig. I.6. As will be shown later, the nondimensional transient response also correlates well with the gas residence times in the reactor bed and the after-bed space. Therefore the results will be presented using residence times rather than length and velocity. In Fig.I.6, the adiabatic flame temperature, pressure, channel diameter, open area fraction and L_c^*/U_{ref}^* are held constant. The solid line in Fig.I.6 gives the response time if the reactor-bed-gas-residence time is the minimum to reach emission goals in steady-state operations. When the combustor inlet temperature is increased, the minimum required reactor-bed-residence time is decreased and the combustor response time is shortened drastically. If a more conservative design is used, i.e. longer bed residence time than is required, the combustor response time is increased for a fixed inlet temperature. The increase is very slight in the beginning when the bed residence time is close to the optimum value but becomes larger as the bed residence time increase further. This implies that a conservative

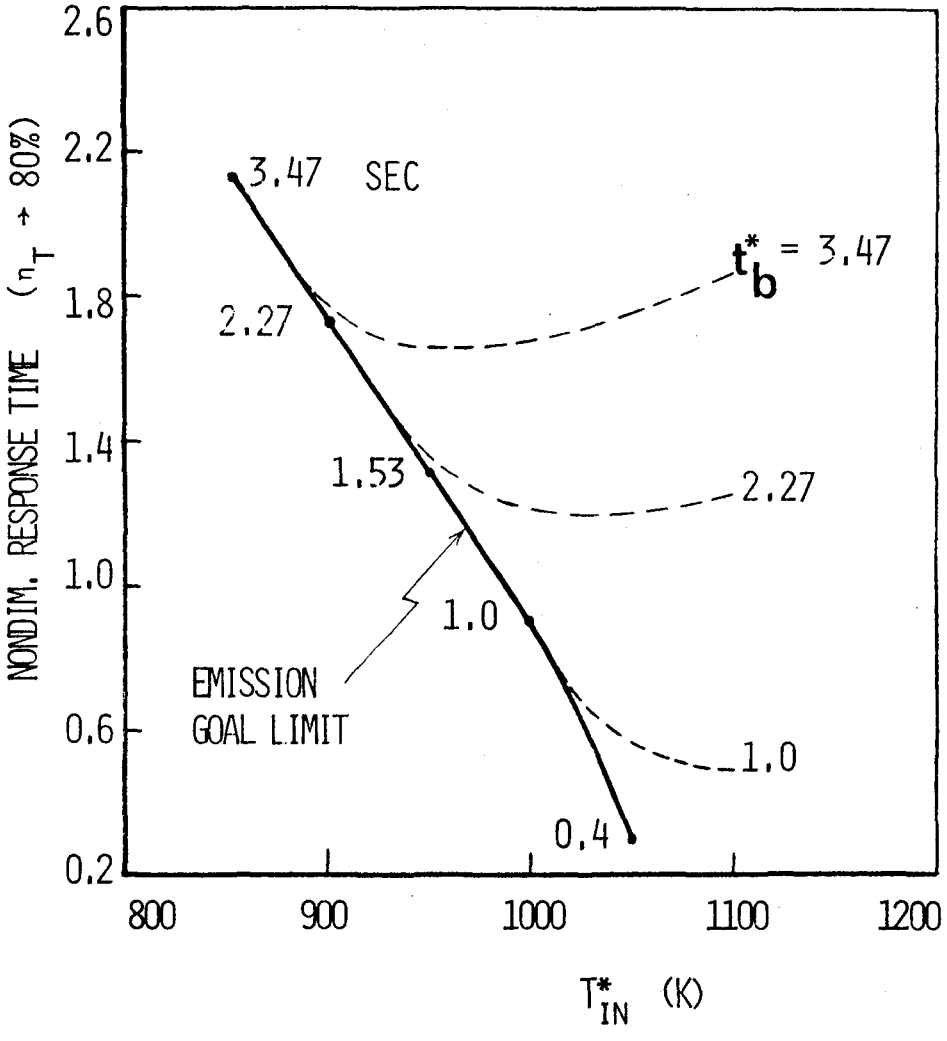

Fig.I.6 Nondimensional response time (η_T goes to 80%) as a function of combustor inlet temperature and reactor bed residence time. L_c^*/U_{ref}^* = 15 msec, T_{af}^* = 1370 K, A^*/A_T^* = .667, d^* = 1.8 mm and p^* = 3 atm.

design with reactor bed length somewhat longer that that of the optimal one will not greatly increase the combustor response time.

Fig.I.7 gives the nondimensional response time as a function of channel hydraulic diameter and flame temperature. For all the calculations in Fig.I.7 the residence time in the catalytic bed, t_b^*, is held constant at 1 milisecond and the residence time in the after-bed space, t_{as}^*, is 13.5 miliseconds. The computation for 1370 K and 1590 K includes different combinations of L^*, L_{as}^*, U_{ref}^* and A^*/A_s^* and it can be seen from Fig.I.7 that the nondimensional response time correlates well with the residence times. *It can, therefore, be concluded that the primary influence of the catalytic bed and after-bed lengths, the approaching gas velocity and the open area percentage is contained in the gas residence times in the catalytic bed and in the after-bed space for both steady and transient operations.*

Fig. I.7 also shows that for a given flame temperature, the nondimensional response time increases with decreasing channel diameter d^*. This, however, does not necessarily mean that the dimensional response time increases with decreasing d^*. If the open area percentage (or equivalently A^*/A_s^*) is fixed, decreasing d^* decreases A_s^* which is used in the reference time scale as defined in Eq (16) and the dimensional response time may actually decrease. Table I.3 gives selected dimensional response times for ceramic and Kanthal metal alloy substrates using the computed results from Fig.I.7. It can be seen that in general the dimensional response time decreases with decreasing channel diameter but the amount of decrease vanishes when the channel diameter becomes too small. In special cases such as the 1590 K flame temperature case, the response time actually reaches a minimum and increases with further diameter decrease.

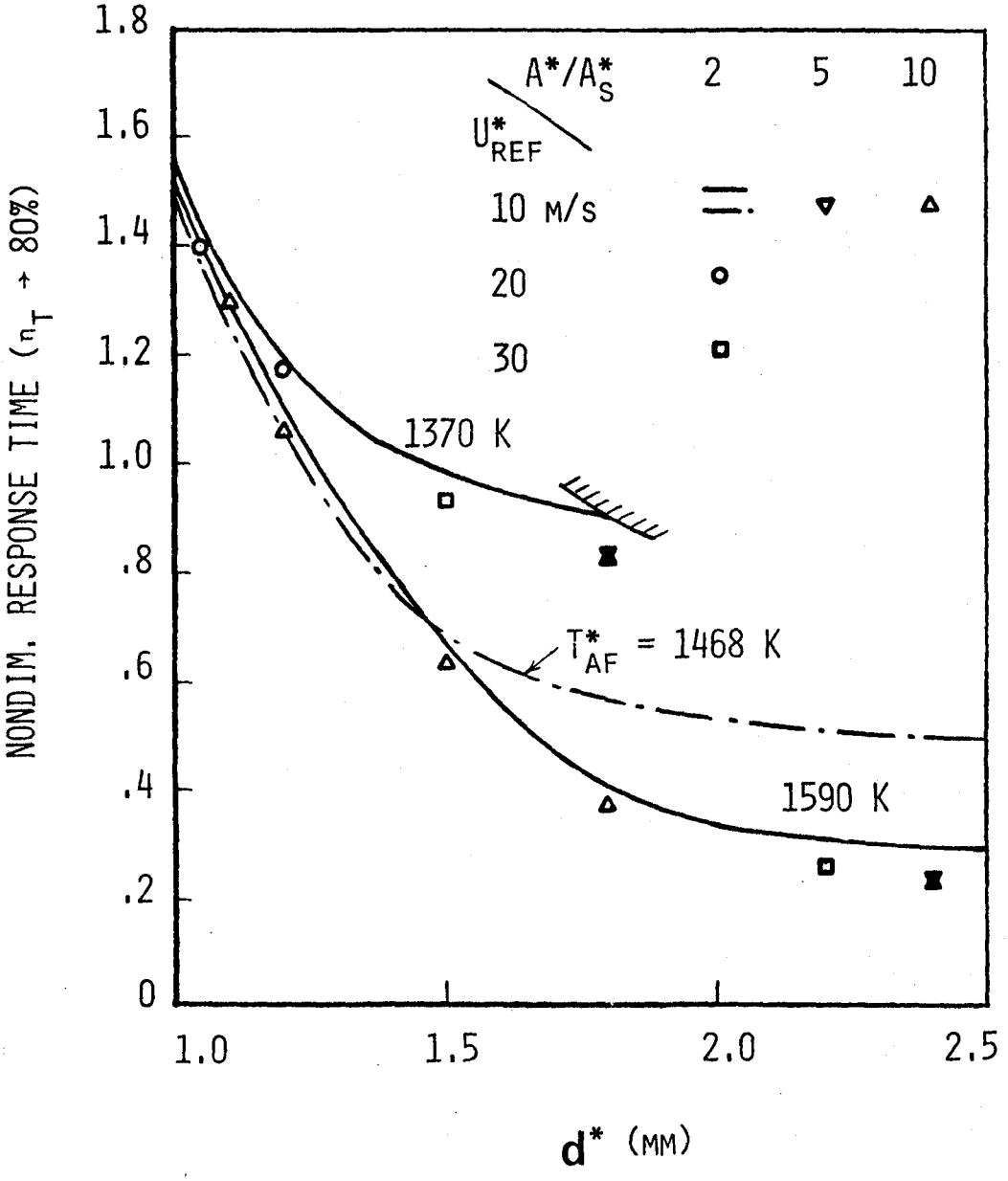

Fig. I.7 Computed nondimensional catalytic combustor response time correlation with gas residence times for various channel diameters and flame temperatures. $p^* = 3$ atm, $t^*_b = 1$ msec, $t^*_{as} = 13.5$ msec, $T^*_{in} = 1000$ K.

Table I.3 Computed Catalytic Combustor Response Time Using Ceramic and Kanthal Metal Substrates.

t^*_b = 1 msec, t^*_{as} = 13.5 msec, p^* = 3 atm, T^*_{in} = 1000 K

T^*_{af} (K)	A^*/A^*_s	d^* (mm)	t^*_r (sec) ceramic	t^*_r (sec) Kanthal alloy
1370	10	1.8	.848	1.52
1370	10	1.0	.451	.807
1468	10	2.5	.909	1.63
1468	10	1.8	.533	.956
1468	10	1.0	.454	.813
1590	10	2.5	.527	.944
1590	10	1.8	.377	.675
1590	10	1.0	.448	.802
1590	5	1.8	.754	1.35
1590	2	1.8	1.88	3.37

If the gas residence times and channel diameter are held constant, varying the open area percentage (or A^*/A_s^*) changes the dimensional response time by a factor of A_s^*/A^*. This is the direct consequence of the correlation between nondimensional response time and residence times as just discussed. Large open area percentage (or thin substrate), therefore, favors fast response.

Fig.7 indicates higher flame temperature shortens the response time for large diameter channel but flame temperature makes little difference in response time for very small diameter channels as all curves converge.

CHAPTER II STEADY STATE COMPUTATION AND COMPARISON WITH EXPERIMENTS

II.1 Three-step Semi-global gas-phase Chemical Reactions

Gas phase reaction studies between hydrocarbons and air in lean mixtures have shown (Dryer and Glassman, 1978) that the hydrocarbon fuel first decomposes into a number of lower hydrocarbons with the simulataneous formation of some water vapor. The combination of these "pyrolysis" steps results in an almost isothermal region after which CO is formed and temperature begins to rise. The carbon monoxide is then oxidized and the reactions are completed. These kinetic studies are very useful for the development of semi-global kinetic schemes.

Two recent catalytic combustion models, by Bracco et al (1980) and T'ien (1980), have utilized the gas phase semi-global modeling concept. The study by T'ien was actually for transient response but a quasisteady gas phase was assumed. The gas phase reactions consist of two semi-global steps; the hydrocarbon reacts with oxygen to form CO and H_2O and CO then reacts with oxygen to form CO_2. On the surface, both hydrocarbon and CO react with oxygen to form CO_2 and or H_2O. The steady-state prediction of that model agrees qualitatively with the experimental trend of CO and hydrocarbon emissions, but a quantitative comparison has not been made. From a pure gas phase reaction point of view, two-step semi-global scheme predicts too high a level of CO in the initial pyrolysis region even though the CO peak level and the decay curve can be made to agree with the experimental data by kinetic parameter adjustment. This early CO appearance problem can be alleviated to a certain

extent by increasing the number of appropriate semi-global gas reaction steps. In the work by Bracco et al (1980), for example, a three-step reaction scheme was used for propane oxidation. Propane (C_3H_8) was assumed to form C_2H_4 first, C_2H_4 to CO next and then CO to CO_2.

For most practical fuels, the pyrolysis intermediates are numerous, and a dominant intermediate species may or may not exist. Since in high inlet temperature operations (T^*_{in} > 800°K), the catalytic combustor length required is limited by the emission level of CO, not hydrocarbons (Anderson, 1980a), it seems reasonable to develop a scheme which gives the correct CO characteristics without being tied down by the uncertain nature of the hydrocarbon intermediates.

In this chapter, the steady-state computation will be based on a three-step gas-phase kinetic scheme. The semi-global reactions are:

(A') $C_nH_m \rightarrow C_nH_m^{(p)}$

$$\frac{d[C_nH_m]}{d\,t^*} = - C_0^* p^{*\gamma_1} [C_nH_m]^{\gamma_2} T^{*\gamma_3} \exp(-E_0^*/RT^*) \qquad (22)$$

(A")

$$C_nH_m^{(p)} + \frac{1}{2}\left(n + \frac{m}{2}\right) O_2 \rightarrow n\ CO + \frac{m}{2}\ H_2O$$

$$\frac{d[C_nH_m^{(p)}]}{d\,t^*} = - C_1^* p^{*\alpha_1} [C_nH_m^{(p)}]^{\alpha_2} [O_2]^{\alpha_3} T^{*\alpha_4} \exp(-E_1^*/RT^*) \qquad (23)$$

(B) $CO + \frac{1}{2} O_2 \rightarrow CO_2$

$$\frac{d[CO]}{d\ t^*} = - C_2^* p^{*\beta_1} [CO]^{\beta_2} [O_2]^{\beta_3} [H_2O]^{\beta_5} T^{*\beta_4} \quad x$$

$$\exp\ (-E_2^*/RT^*) \qquad (24)$$

In reaction (A'), Eq. (22), the original hydrocarbon fuel forms the "pyrolyzed hydrocarbon", $C_n H_m^{(p)}$, in an <u>isothermal</u> reaction. The "pyrolyzed hydrocarbon" then reacts with oxygen to form CO and H_2O in reaction (A"). In reaction (B), CO is oxidized to CO_2. The introduction of reaction (A') serves to decrease the amount of early CO appearance as found using the two-step model. The identity of $C_n H_m^{(P)}$ is of no great consequence for the purpose of this modeling work, if the mass diffusion coefficient is properly evaluated. For convenience, in the present calculation we take $C_n H_m^{(P)}$ to have the same n and m as the original fuel.

Corresponding to the reactions given by Eqs. (22-24), the species equations are:

Original Hydrocarbon:

$$\rho u \frac{d\mathcal{Y}_{HC}}{dx} + J_{D_1}(\mathcal{Y}_{HC} - \mathcal{Y}_{HC,s}) = - W_o \qquad (25)$$

"pyrolyzed" Hydrocarbon:

$$\rho u \frac{d\mathcal{Y}_{HC}^{(p)}}{dx} + J_{D1} \left(\mathcal{Y}_{HC}^{(p)} - \mathcal{Y}_{HC,s}^{(p)} \right) = w_o - w_1 \tag{26}$$

Carbon monoxide:

$$\rho u \frac{d\mathcal{Y}_{CO}}{dx} + J_{D2} \left(\mathcal{Y}_{CO} - \mathcal{Y}_{CO,s} \right) = w_1 C_n - w_2 \tag{27}$$

Oxygen:

$$\mathcal{Y}_{O_2} = 1 - \phi \left(1 - \mathcal{Y}_{THC}\right) + \frac{1}{2} \mathcal{Y}_{CO} \left(\frac{Y_{HC}(o)}{Y_{O_2}(o)} \frac{W_{O_2}}{W_{CO}} \right) \tag{28}$$

where

$$\mathcal{Y}_{THC} = \mathcal{Y}_{HC} + \mathcal{Y}_{HC}^{(p)}$$

The reaction rates are given by

$$w_o = B_o p^{\gamma_1} \rho^{\gamma_2} T^{\gamma_3} \mathcal{Y}_{HC}^{\gamma_2} \exp(-E_o/T) \tag{29}$$

$$w_1 = B_1 p^{\alpha_1} \rho^{(\alpha_2 + \alpha_3)} T^{\alpha_4} \mathcal{Y}_{HC}^{\alpha_2} \mathcal{Y}_{O_2}^{\alpha_3} \exp(-E_1/T) \tag{30}$$

$$w_2 = B_2 \, p^{\beta_1} \rho^{(\beta_2+\beta_3+\beta_5)} T^{\beta_4} \mathcal{Y}_{CO}^{\beta_2} \mathcal{Y}_{O_2}^{\beta_3} Y_{H_2O}^{\beta_5} \exp(-E_2/T) \tag{31}$$

and

$$Y_{H_2O}(x) = \frac{m}{2} \frac{W_{H_2O}}{W_{HC}} Y_{HC}(o) \left[\mathcal{Y}_{THC}(o) - \mathcal{Y}_{THC}(x) \right] \tag{32}$$

Three global catalytic surface reactions are assumed to occur on the surface. They are:

$$(C')\ C_nH_m + (n+\tfrac{m}{4})\ O_2 \rightarrow nCO_2 + \tfrac{m}{2}\ H_2O \tag{33}$$

with the corresponding surface rate J_3^* given by

$$J_3^* = C_3^*\ [C_nH_m]_s\ \exp\ (-E_3^*/RT_s^*)$$

$$(C'')\ C_nH_m^{(p)} + (n+\tfrac{m}{4})O_2 \rightarrow nCO_2 + \tfrac{m}{2}\ H_2O \tag{34}$$

$$\text{with } J_4^* = C_3^*[C_nH_m^{(p)}]_s\ \exp\ (-E_3^*/RT_s^*)$$

$$(D)\quad CO + \frac{1}{2}\ O_2 \rightarrow CO_2 \tag{35}$$

$$\text{with } J_5^* = C_4^*[CO]_s\ \exp\ (-E_4^*/RT_s^*)$$

Other equations are similar to those in Chapter I. The steady solution is obtained from the transient combustion code as discussed in Chapter I.

II.2 Computed Results

The design parameters of a catalytic combustor include the catalytic bed length, the after-bed reaction distance, the channel hydraulic diameter, the open area percentage, the catalyst variables (catalyst type, loading density, washcoat type) and staging arrangements (graded cell, for example). The operating parameters include inlet temperature and pressure, the approaching (reference) mixture velocity, the fuel/air equivalence ratio or the adiabatic flame temperature and fuel types. An exhaustive parametric study will not be practical for this report. Instead, selected computations are presented. Since emphasis is placed on automotive gas turbine application, we are most interested in higher inlet temperature, above atmospheric pressure and high reference velocity operations with thin substrate and large open area percentage design. The total combustor length (bed plus after-bed) required to meet the emission goal (13.6 g CO/kg fuel, 1.64 g THC/kg fuel) as a function of these parameters is the main output of the model calculation.

The chosen fuel is No. 2 Diesel which was used by Anderson (1977a, 1978, 1980a). Its hydrogen-carbon atom ratio is 1.8 with 27.55% aromatics. The molecular weight is taken to be 138 for the purpose of estimating the diffusion coefficient which is assumed to vary as one over the square root of molecular weight. Other properties can be found in Anderson (1977a). The catalytic combustor used for reference calculation is the one by Matthey Bishop which was also described by Anderson (1980a) (MBI-2.5 and MBI-5.4). The values of kinetic parameters are listed in Table II.1. Expressions in Reactions A" to D are taken from Edelman and Fortune (1969), Dryer and Glassman (1973), Marteney (1979) and Kuo and Morgan (1971) respectively, all with adjusted pre-exponential

Table II.1 Chemical Kinetic Constants
(for Chapter II)

Reaction (A')	Reaction (A")	Reaction (B)	Reactions (C')(C")	Reaction (D)
$C_o^* = 1.6 \times 10^6$	$C_1^* = 1.8 \times 10^5$	$C_2^* p^{*\beta_1} = .54 \times 10^{14}$ (at 3 atm)	$C_3^* = 1.5 \times 10^4$	$C_4^* = 10^5$
$\gamma_1 = 0$	$\alpha_1 = 0.3$		$E_3^* = 10$ (kcal/mole)	$E_4^* = 17.8$ (kcal/mole)
$\gamma_2 = 0.5$	$\alpha_2 = 0.5$	$\beta_2 = 1$		
$\gamma_3 = 0$	$\alpha_3 = 1$	$\beta_3 = 0.25$		
	$\alpha_4 = 1$	$\beta_4 = 0$		
$E_o^* = 34$ (kcal/mole)	$E_1^* = 24$ (kcal/mole)	$\beta_5 = 0.5$		
		$E_2^* = 40$ (kcal/mole)		

factors. The calculated results are not very sensitive to catalytic kinetic parameters indicating mass transfer dominates the surface reactions. The choice of gas-phase hydrocarbon oxidation kinetic constants deserves some explanation, since kinetic rates for No. 2 Diesel fuel are hard to find. Ignition delay times as a function of initial temperature, however, do exist for long chain and cyclic hydrocarbons (Dryer and Glassman, 1978, Edelman, 1978), which are the ingredients of the Diesel fuel. The ignition delay time of No. 2 Diesel is assumed to be the arithmetic mean of its ingredients. Model calculations are then performed for pure gas phase reactions and the ratio of calculated hydrocarbons disappearance times as a function of initial temperature is taken to be proportional to the ratio of ignition delay times as indicated in Fig. II.1. This provides some measure for the correct temperature dependence in the gas kinetic parameters for the diesel fuel. The use of "hydrocarbon disappearance time" in this comparison reflects the difficulty of identifying ignition time in the theoretical study. The pre-exponential factor in reaction (B) is adjusted to fit the CO decay data of Anderson (1980a).

The model calculations for the catalytic combustors will be presented next.

Effects of Catalytic Bed Length, Downstream Reaction Distance, Reference Velocity and Adiabatic Flame Temperature

Figure II.2 shows the detailed profiles of two cases; one with a 5-cm bed and the other with a 2.5-cm bed. If we look at the 5-cm case first, we see when mixture enters into the reactor channel, the fuel is quickly consumed on the surface by catalytic reaction, the surface temperature starts from a low value (T_s = 1.106), due to the fast heat and mass transfer rates at the entrance region, and rises sharply away from the channel entrance. The gas

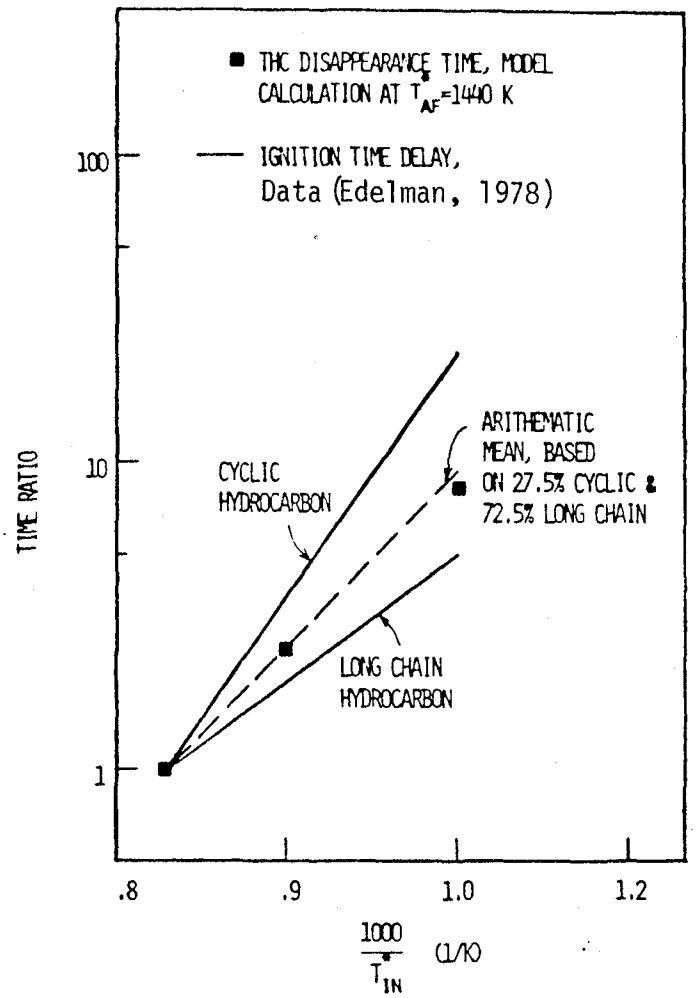

Fig. II.1 Comparison of temperature dependence for the computed disappearance time (nondimensional) of Diesel No. 2 fuel with Ignition Delay Data (Edelman, 1978). Reference time is taken at 1200 K.

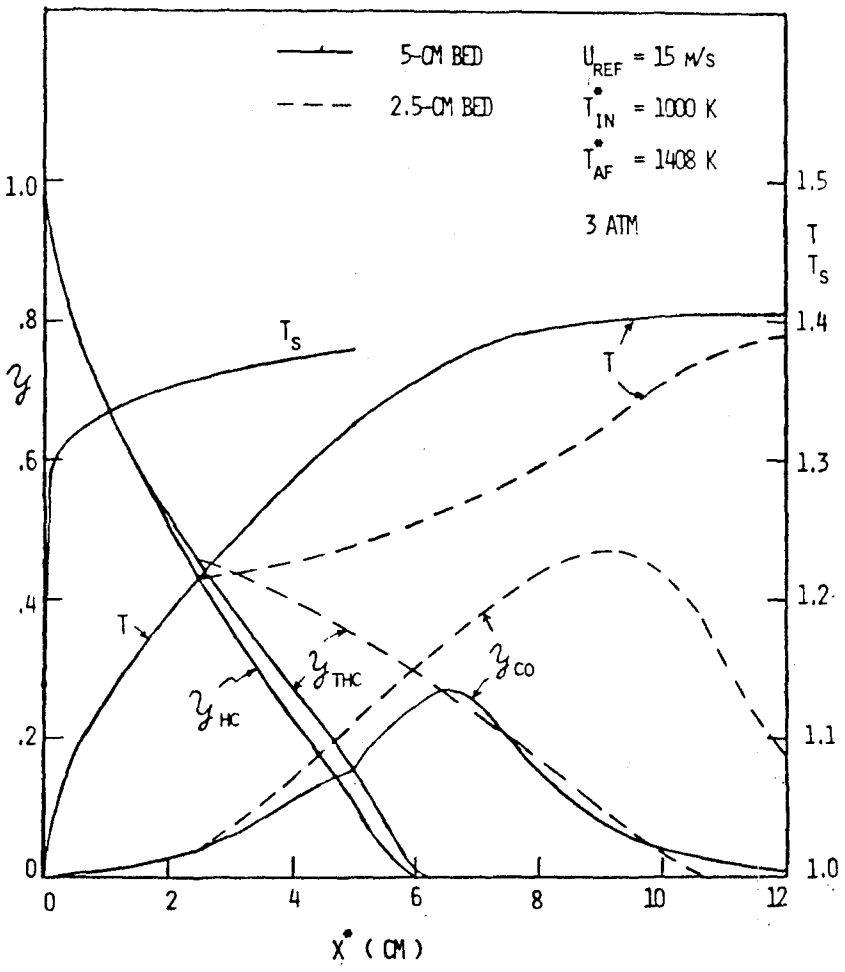

Fig. II.2 Computed temperature and species profiles for two similar catalytic combustors with different bed lengths, A^*/A^*_T = 0.93 and d^* = 1.382 mm.

temperature begins to rise due to the heat transfer from the substrate and when T reaches 1.15, gas-phase reaction is initiated and the hydrocarbon fuel is converted to the "pyrolyzed hydrocarbon,", which is equal to the difference between $\mathcal{Y}_{THC}$ (total hydrocarbon) and $\mathcal{Y}_{HC}$ (original hydrocarbon). At the same time, CO, which is produced only in the gas-phase, begins to rise. The carbon monoxide in turn is consumed by both gas-phase and surface reactions to form CO_2 until the bed exit is reached. After the exit, CO is consumed by gas-phase reaction only so a slope discontinuity of the CO curve occurs at $x^* = 5$ cm. Similar discontinuity can be found in temperature and hydrocarbons, although in the latter case, it is not very apparent. If at the bed exit the gas temperature is high enough, the gas-phase reaction will continue at a high rate and adiabatic flame temperature is reached at $x^* = 12$ cm. As shown in Fig. II.2, a CO peak occurs when its production and oxidation rates become equal.

If the catalytic bed is cut short at 2.5 cm. as shown in Fig. II.2, the total hydrocarbon ($\mathcal{Y}_{THC}$) oxidation rate decreases suddenly at the bed exit (2.5 cm) due to the absence of surface reaction. Since the gas temperature is not yet high enough, the gas-phase reaction downstream proceeds slowyly as shown by the slower increase of gas temperature. Because a larger fraction of the hydrocarbon fuel has to be consumed in the gas-phase reaction, higher CO peak occurs and the total combustor length required to reach the emission goal is accordingly longer than the case with longer catalytic bed.

It was shown in Chapter I that the effects of catalytic bed length, after-bed distance, gas velocity and open area percentage could be correlated using reference gas residence times in the reactor bed and in the after-

bed space. For a fixed open area fraction, this correlation is simplified and can be expressed by the ratios of lengths over the reference velocity as given in Fig. II.3. For a fixed "gas residence time" in the bed (L^*/U^*_{ref}), there is a corresponding minimum combustor residence time (L^*_{EG}/U^*_{ref}) for emissions goals to be satisfied. Although the residence time correlation is natural for gas-phase reactions, it is less obvious for surface reactions. The validity of this type of correlation is independent of the gas kinetic schemes used as illustrated here and in Chapter I where two-step kinetics and different sets of catalytic parameters were employed.

Fig. II.3 shows that as the catalytic bed length increases, the required combustor length decreases. This may lead one to choose a design which is all reactor bed without the downstream gas reaction space. However, as discussed in Chapter I, in many catalytic combustor applications (e.g., transportation engines), a fast combustor response is required. Longer reactor bed results in a longer response time due to the larger substrate thermal inertia. Therfore, certain compromises may have to be made between steady and nonsteady considerations. Take Fig. II.3, for example, one may want to choose a bed residence time of 4 milliseconds instead of 6 milliseconds. This increases the total combustor length by 15% but reduces the response time by 30%. As the inlet temperature becomes higher, as preferred by the automotive gas turbine design, the required reactor bed will be drastically reduced, leaving most reactions to occur in the gas-phase. A shorter reactor bed also decreases the pressure loss.

The importance of downstream gas-phase reactions has been recognized by Anderson as demonstrated in much of his work (Anderson, 1977b, 1980a, T'ien and Anderson, 1979). Figure II.4 compares the model calculation with his recent data (Anderson, 1980a) on CO emission index as a function of downstream

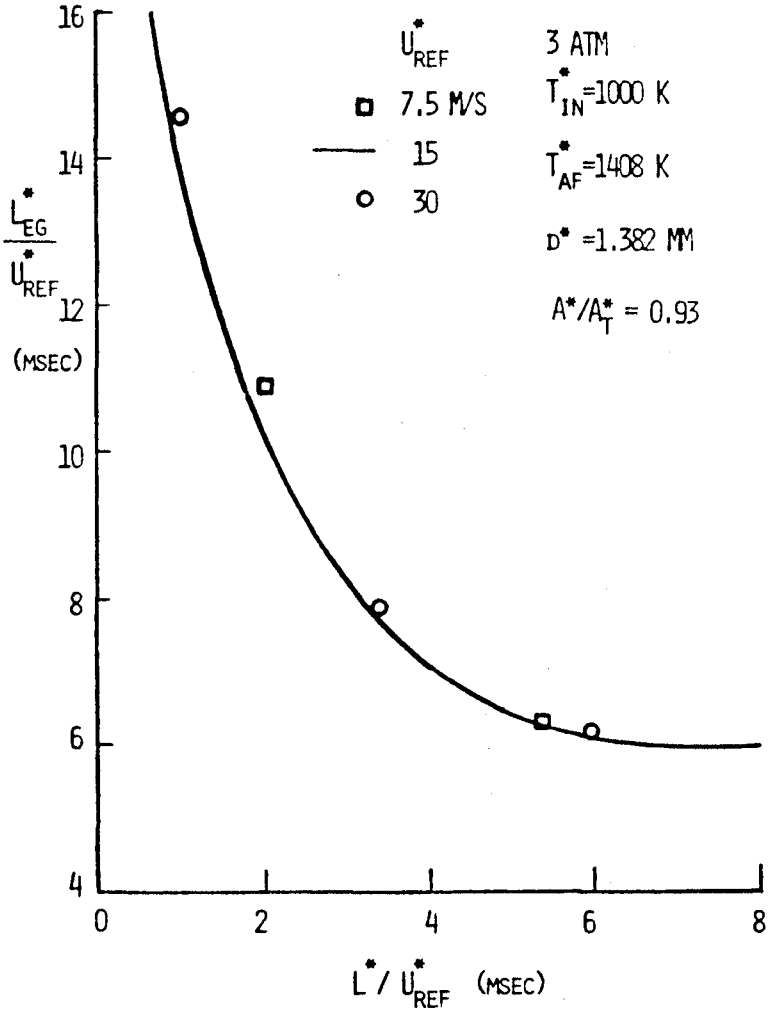

Fig. II.3 Computed "residence time" correlation: total residence time in combustor (bed plus after-bed) to reach emission goals vs. residence time in catalytic beds.

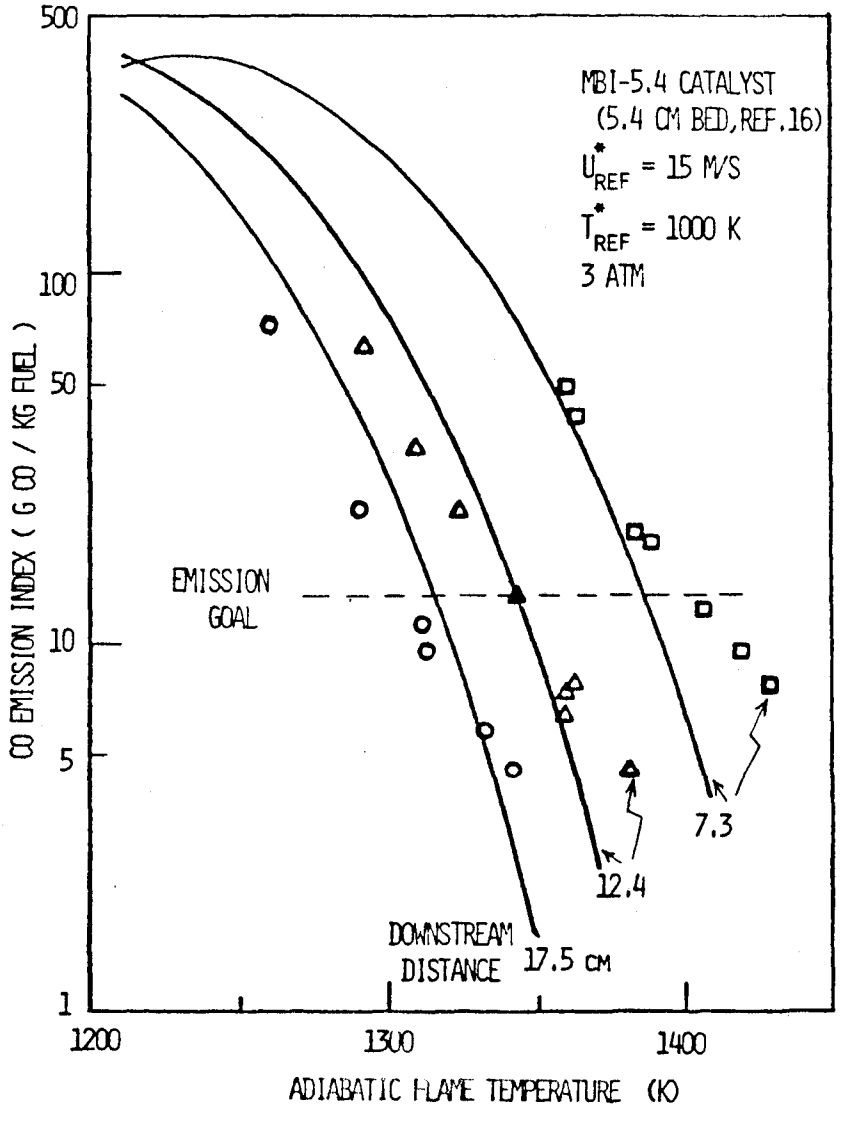

Fig . II.4 CO emission index vs. adiabatic flame temperature: comparison of model calculation with Anderson's data (1980a).

reaction distance and adiabatic flame temperature. Figure II.5 compares the minimum operating flame temperature vs. the downstream reaction distance for two bed lengths and two velocities. The comparison between the model and data is reasonably good within the range of parameters varied.

The appearance of CO peak as indicated in Fig. II.2 has been reported in previous experimental work (T'ien and Anderson, 1979, Bracco et al, 1980).

Effects of Inlet Temperature and Pressure

Figure II.6 shows the computed combustion efficiency as a function of adiabatic flame temperature for three inlet temperatures and two pressures at three different downstream locations. For a fixed pressure and adiabatic flame temperature, higher inlet temperature results in a higher efficiency at all three downstream positions. This is consistent with the experimental trend found by Anderson (1978). With higher inlet temperature, the gas-phase reaction is initiated earlier which results in a higher efficiency at a fixed location. However, as more residence time is given to the mixture, the difference in efficiency diminishes as can be seen from curves at different locations in Figure II.6.

From Fig. II.6, for inlet temperature of 1000 K, the combustion efficiency at 3 atm is always higher than that at 6 atm. This is because of the faster mass diffusion rate at lower pressure. For 1100 K inlet temperature, however, a portion of the 6 atm efficiency curve is higher than that of the 3 atm case as can be seen in Fig. II.6(b) and (c). This reversal phenomenon was first reported by Anderson (1978) who suggested that this was due to the competition between gas-phase and surface reactions. This model calculation

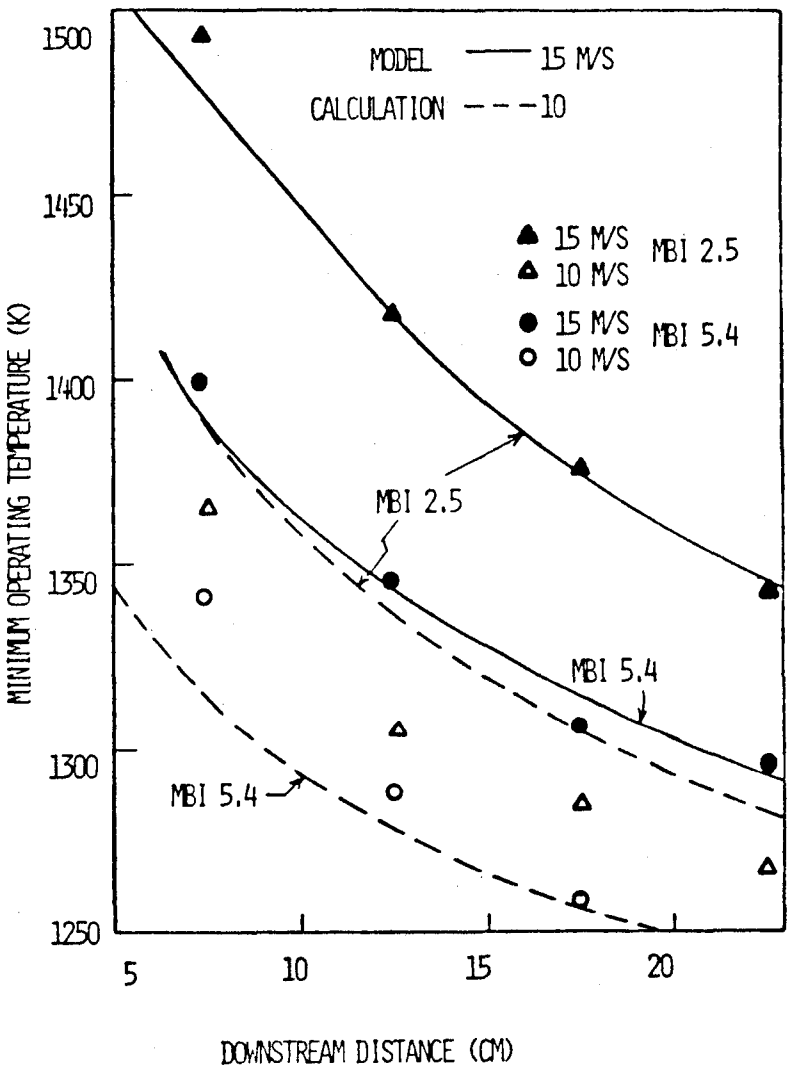

Fig. II.5 Minimum operating flame temperature (to reach emission goals) vs. downstream reaction distance: comparison of model calculation with Anderson's data (1980a).

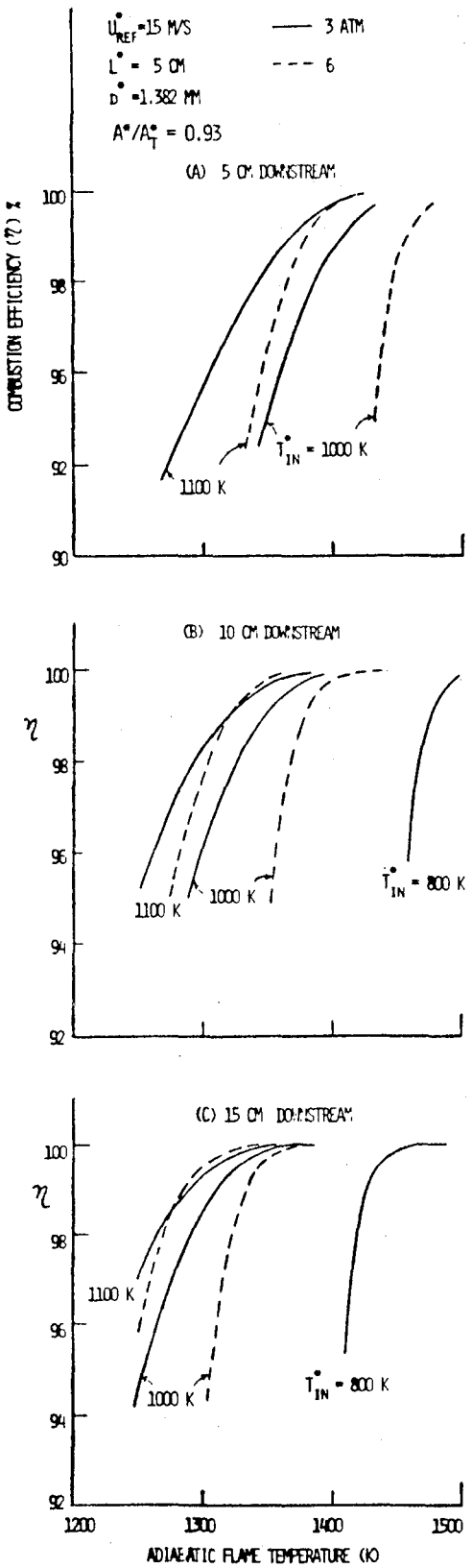

Fig. II.6 Combustion efficiency vs. adiabatic flame temperature for different inlet temperature and pressure at three downstream locations.

supports this interpretation. High temperature and pressure support fast gas-phase reactions, but high pressure also retards surface reaction through slower mass diffusion rate. Taking the case of 1100 K inlet temperature and 1320 K adiabatic flame temperature for example: at the bed exit, the 6 atm case has a lower efficiency than the 3 atm case because inside the reactor channel, surface reaction dominates. At downstream distance of 5 cm, the 6 atm case still has lower efficiency. But at 10 cm downstream, the two efficiencies become equal and at 15 cm downstream 6 atm has a higher efficiency. Since only gas-phase reaction exists in the after-bed space, the efficiency reversal occurs when the gas-phase reactions overpower the upstream influence of surface reactions.

SUMMARY

A transient model of monolith catalytic combustor is presented in this work. The model assumes a quasisteady gas phase and a thermally-thin solid with the substrate thermal inertia responsible for the combustor response time delay. In the gas-phase treatment, several quasi-global chemical reactions are assumed which are capable of describing CO and unburnt hydrocarbon emissions in fuel-lean operations. By neglecting heat conduction along the flow direction in the gas and the solid in high speed approaching flows, the system of differential equations describing the combustor transient is simplified and Runge-Kutta integration scheme is applicable. The resulting computation scheme is highly efficient in computational time and is suitable for parametric calculation for both steady states and transients.

In the steady-state computation presented, the influence of selected operating and design parameters on the minimum combustor length is studied. Special attention is given to the effect of after-bed gas phase reaction space. Comparison with the data by Anderson indicates that the model is able to describe all the salient features found in the experiments including the appearance of CO peak and the efficiency reversal phenomena at high inlet temperature and pressure. Quantitative agreement with CO emission data is possible if a certain degree of rate constants adjustment is made.

The model computation also suggests that for determining the condition of achieving the steady-state emission goals, the gas residence times in the catalytic bed and in the after-bed space are the similarity parameters absorbing the influence of catalytic bed and after-bed lengths, the gas velocity and the open area fraction of the catalytic element. Likewise, the nondimensional

response time and the gas residence times are the proper similarity parameters in transient operations. A consequence of this is that the dimensional response time is proportional to the substrate crossectional area A_s^* (all other parameters fixed) and so a thin substrate is necessary for fast response.

The computed time history provides an understanding of how a catalytic combustor responds to an upstream condition change. The leading edge of the substrate is the first to respond to an upstream variation, say, a change of fuel flow rate. The leading edge is closer to the source of variation and the mass transfer rate is higher in the flow entrance region of the gas channel. As a result, the surface fuel concentration is perturbed first which, through the surface reaction, produces a surface temperature change. Heat transfer across the flow channel then causes the gas temperature to vary and this disturbance propagates downstream by convection. Since, the downstream part of the substrate always responds to the upstream substrate temperature variation, it is not difficult to see from the above description that a combustor with a longer catalytic bed residence time will take a longer time to reach a new equilibrium state.

The model calculation also shows that higher combustor inlet temperature and adiabatic flame temperature shorten the response time. Smaller channel hydraulic diameter usually results in a faster response but there are exceptions. Since the requirements for faster transient response do not always coincide with the optimal steady-state design conditions, for applications where transient characteristics are important, both steady and transient studies have to be made simultaneously so that a good compromising design can be found.

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Nomenclature

A^* crossectional area of one gas channel

A_s^* substrate cross-sectional area associated with one gas channel, see Fig. 1

$A_T^* = A^* + A_s^*$, total crossectional area of one cell unit

$$B_0 = \frac{L^*}{U^*(0)} \frac{1}{\rho^*(0)} \frac{1}{Y_{HC}(0)} C_0^* \, p^*(0)^{\gamma_1} \rho^*(0)^{\gamma_2} T^*(0)^{\gamma_3} Y_{HC}(0)^{\gamma_2} W_{HC}^{(1-\gamma_2)}$$

$$B_1 = \frac{L^*}{U^*(0,0)} \frac{1}{\rho^*(0,0)} \frac{1}{Y_{HC}(0,0)} C_1^* \, p^*_{(0,0)}{}^{\alpha_1} \rho^*_{(0,0)}{}^{(\alpha_2+\alpha_3)} T^*_{(0,0)}{}^{\alpha_4} Y_{HC}(0,0)^{\alpha_2} Y_{O2}(0,0)^{\alpha_3} \times W_{HC}^{(1-\alpha_2)} W_{O2}^{-\alpha_3}$$

$$B_2 = \frac{L^*}{U^*(0,0)} \frac{1}{\rho^*(0,0)} \frac{1}{Y_{HC}(0,0)} C_2^* \, p^*(0,0)^{\beta_1} \rho^*(0,0)^{(\beta_2+\beta_3+\beta_5)} T^*_{(0,0)}{}^{\beta_4} Y_{HC}^{\beta_2}(0,0) \times Y_{O2}^{\beta_3}(0,0) W_{CO}^{(1-\beta_2)} W_{O2}^{-\beta_3} W_{H_2O}^{-\beta_5}$$

$$B_3 = C_3^* \, d^* \, / \, \alpha^* W_{HC} Nu_\infty$$

$$B_4 = C_4^* \, d^* \, / \, \alpha^* W_{CO} Nu_\infty$$

$$C_n = n \, W_{CO} \, / \, W_{HC}$$

C_s^* specific heat of substrate

C_p^* gas specific heat

d^* catalytic monolith combustor channel equivalent diameter

d_s^* half thickness of the substrate

E^* activation energy

J_3^* mass consumption rate of hydrocarbons per unit surface area through reaction (C)

J_4^* mass consumption rate of CO per unit surface area through reaction (D)

$$J_{Di} = J_H \, (Le_i)^{2/3}$$

$$J_H = 4 \, Nu_x (\alpha^*(0,0)/d^{*2})(L^*/u^*(0,0)(k^*/k^*(0,0)$$

k^* heat conductivity of the gas

L^* catalytic bed length

L^*_{as} length of after-bed downstream gas phase reaction space

L^*_c total combustor length (catalytic reactor length plus after-bed downstream gas reaction distance)

L^*_{EG} total combustor length (catalytic bed plus after-bed space) required to meet emission goals

Le_1 Lewis number for hydrocarbon gas in air

Le_2 Lewis number for CO in air

m number of hydrogen atom in C_nH_m

n number of carbon atom in C_nH_m

Nu_x Nusselt number at x

Nu_∞ Nusselt number for fully developed flow

p = $p^*/p^*(0,0)$, nondimensional pressure

q_1 = $q_1^*/C_p^*T^*(0,0)$, nondimensional heat of combustion per unit mass of C_nH_m in reaction A

q_2 = $q_2^*/C_p^*T^*(0,0)$, nondimensional heat of combustion per unit mass of CO in reaction B

q_3 = $q_3^*/C_p^*T^*(0,0)$, nondimensional heat of combustion per unit mass of C_nH_m in reaction C

q_4 = $q_4^*/C_p^*T^*(0,0)$, nondimensional heat of combustion per unit mass of CO in reaction D, same as q_2

r_{nk} see Eq. (17)

S^* circumferential length of one channel crossection ($= \pi d^*$)

T = $T^*/T^*(0,0)$, nondimensional gas temperature

T_s = $T_s^*/T^*(0,0)$, nondimensional substrate temperature

T^*_{af} adiabatic flame temperature

T^*_{in} combustor inlet temperature

$t = t^*/\tau^*$, nondimensional time

$t^*_b = (L^*/U^*_{ref})\ (A^*/A^*_T)$, reference gas residence time in the catalytic combustor bed

$t^*_{as} = L^*_{as}/U^*_{ref}$, reference gas residence time in the after-bed space

t^*_{ch} characteristic transient response time ($\eta_T \rightarrow 80\%$)

t^*_{EG} Minimum total combustor gas residence time ($t^*_b + t^*_{as}$) needed to reach emission goals

$u = u^*/u^*(0,0)$, nondimensional flow velocity

u^*_{ref} reference gas velocity, measured at upstream of catalytic bed

W_i molecular weight of species i

w_i chemical reaction rate

$x = x^*/L^*$, nondimensional axial distance measured from catalytic bed entrance to downstream

Y_i mass fraction of species i

$\gamma_{CO} = Y_{CO}/Y_{HC}(0,0)$

$\gamma_{O2} = Y_{O2}/Y_{O2}(0,0)$

$\gamma_{HC} = Y_{HC}/Y_{HC}(0,0)$

$\gamma^{(p)}_{HC} = Y^{(p)}_{HC}/Y_{HC}(0)$

$\gamma_{THC} = \gamma_{HC} + \gamma^{(p)}_{HC}$

α^*	thermal diffusivity of gas
α_i	rate exponent, see Eqs (1) and (23)
β	rate constant, see Eq. (22)
β_i	rate exponent, see Eqs (2) and (24)
γ_i	rate exponent, see Eq (22)
ρ^*	gas density
ρ_s^*	substrate density
τ^*	characteristic substrate heat-up time, see Eq. (16)
η_{CB}	carbon-balanced efficiency
η_T	combustion efficiency based on temperature difference
$[\ ]$	concentration, g-mole/c.c.

Subscript

s	surface

Superscript

*	dimensional quantity

APPENDIX I

LISTING OF COMPUTER PROGRAMS FOR CHAPTER I

The numerical computations were performed using an interactive VAX - 11/780 computer. FORTRAN language was used in writing the main program (e.g. IGNITION. FOR; 17) and the data program (e.g. BLOCK. FOR; 31). They were then compiled to form the objective programmes (e.g. IGNITION. OBJ; ** and BLOCK. OBJ; **). The two objective programmes were then linked together to form an executable program (e.g. IGNITION. EXE; 10). In performing a calculation, only the executable is needed.

The BLOCK program stores most of the data which are not likely to be changed from one calculation to the other, while the most frequently varied input data will be read in in each computer run. If the data stored in the BLOCK program are to be changed, the FORTRAN BLOCK program has to be modified (edited), re-compiled and linked with the main program to form a new executable program.

In the following,the FORTRAN programmes (IGNITION. FOR; 17 and BLOCK. FOR; 31) are listed together with a sample calculation showing input and output data.

The IGNITION program is presently set up to perform the start-up transient. With minor modification, it can read in any prescribed initial condition and to calculate the corresponding unsteady response. Given enough computational time, the IGNITION program will also result in the steady-state profiles.

More detailed instrictions (for IGNITION. FOR; 17):

1. The number of grid points used should be less than 300. If more than 300 points are needed, line 600 has to be changed.
2. Read-in data (lines 10900 - 12300):
   XPHI = ϕ= fuel-air equivalence ratio

TI = T (0,0) = upstream, initial temperature (K)

XPI = P(0,0) = upstream, initial pressure (Atm.)

UIUS = U_{ref} = upstream (outside of the bed) initial gas velocity (m/s)

XLS = reference length (m), suggested to use 0.1 m (10 cm)

DS = d* = channel hydraulic diameter (m)

AOAS = A^*/A^*_s = open-to-close area ratio

D_X = nondimensional step size in X (space). It is nondimensionalized by XLS. So if XLS = 0.1 m and DX = 0.01, dimensional step size is 0.001 m or 1 mm.

DT = nondimensional time step size

TMAX = maximum nondimensional time allowed for computation

IPRINT = time interval for printing out transient profiles. For example, if DT = .01 and IPRINT = 25, Output will be printed out every t = 0.25.

N = number of grid points (in X direction) in the catalytic bed. The nondimensional catalytic bed length is given by (N-1) x (DX). For example, if N = 51, DX = .01, then the nondimensional bed length is equal to 0.5. If XLS = .1 m, then the dimensional bed length is .05 m (5 cm).

NAS = number of grid points (in X-direction) in the downstream after-bed space. The length of the downstream distance can be calculated in a similar manner as in the above.

C1, C2, C3, C4 = C_1, C_2, C_3, C_4 (See Table I.2)

IT = interval in X for printout. For example, if DX = 0.01 IT = 5, the printout will be at X = 0, 0.05, 0.1, 0.15, . . . etc.

3. Those data which are not read in will be defined by the BLOCK program.

4. Some Symbol Definitions:

PR = Prandtl number of air

REY = Reynolds number based on channel diameter and upstream velocity

ES,S = E_1*, E_2*, E_3*, E_4* (See Table I.2)

E,S = E_1, E_2, E_3, E_4

C,S = C_1*, C_2*, C_3*, C_4* (See Table I.2)

GC = gas constant (joule/kg K)

XLEW1 = Lewis number for C_nH_m in mixture

XLEW2 = Lewis number for CO in mixture

ROI = initial, upstream (I.U.) gas density (kg/m^3)

XKI = I.U. gas heat conductivity (cal/m sec K)

CP = specific heat of gas at constant pressure (cal/kg K)

ALPHA = I.U. gas diffusivity (m^2/sec)

TS = T_s

YFS = $y_{HC,s}$

YCS = $y_{CO,s}$ YO = y_{O_2}

YF = y_{HC} TMAX = Maximum time for computation

YC = y_{CO}

5. Output data (lines 40300 to 42200)

The following quantities are printed out as a function of axial distance and time:

Nondimensional gas and surface temperatures, Emission indices (x1000) of hydrocarbon fuel and CO (both in the gas phase and on the surface) and carbon-balanced and thermal efficiencies.

```
C
C     ****************************************************************
C     *******CATALYTIC COMBUSTOR START-UP TRANSIENT*******************
C     ****************************************************************
C
      PARAMETER NX=300
      COMMON /ACTI/ES1,ES2,ES3,ES4
      COMMON /MOLEQ/  WHC, WCO, WO2, WH2O
      COMMON /TH1/XM, XM, G1S,G2S
      COMMON /TH2/ CP, GC, XPR
      COMMON /UPS1/ YCI, YCI
      COMMON /IN1/TS,YFS,YCS
C
      DIMENSION YF(NX), T(NX), TS(NX), YO(NX), YFS(NX), RO(NX), U(NX)
      DIMENSION XKY(4), XKT(4), XKTS(4), XKC(4), YC(NX), YCS(NX)
      DIMENSION  XJH(NX), XJD1(NX), XJD2(NX), YH2O(NX)    ,XP(NX)
      DIMENSION EFF(NX), RNK(NX),EFFT(NX)
C
    7 FORMAT (4E20.10)
    8 FORMAT (I4)
    9 FORMAT (1H0,'SOLID TEMPERATURE (TS)'/)
   10 FORMAT (6F12.6)
   11 FORMAT (1H0,'SURFACE HC MASS FRACTION (YFS)'/)
   12 FORMAT (//)
   13 FORMAT (1H0,'GAS TEMPERATURE (T)'/)
   14 FORMAT (1H0,'CNHM MASS FRACTION (YF)'/)
   15 FORMAT(1H0,'YO(UPST,IN1) =',F10.6,5X,'YF(UPST,IN1)=',F10.7
     1,5X,'EQUI RATIO ='F15.9//)
   17 FORMAT (1H0,'G1=',F15.7,5X,'G2=', F15.7,5X,'DX=',F15.7,5X,'DT=',
     1F15.7//)
   18 FORMAT (1H0,'N=',I10//)
   19 FORMAT (1H0,'INITIAL CONDITIONS (TS)',/)
   20 FORMAT (1H0,'TMAX = ',F15.8)
   21 FORMAT (1H0,'NO. OF GRID POINT =',2I10//)
   22 FORMAT (1H0,'TIME=',F15.8,5X,'KOUNT=',I10/)
   23 FORMAT (///)
   24 FORMAT (10E12.5)
   25 FORMAT (1H0,'INITIAL CONDITIONS (YFS)',/)
   26 FORMAT (1H0,'XJH'/)
   31 FORMAT (1H0,' CO MASS FRACTION (YC)'/)
   32 FORMAT (1H0,'SURFACE CO MASS FRACTION (YCS)'/)
   33 FORMAT (1H0,'INITIAL CONDITIONS (YCS)',/)
   34 FORMAT (1H0,' ES,S = ',6F12.6/)
   35 FORMAT (1H0,'  C,S = ',4E20.10/)
   36 FORMAT (1H0,'  A,S = ',6F12.6/)
   37 FORMAT (1H0,' BE,S = ',6F12.6/)
   41 FORMAT (1H0,' YCO =',/)
   42 FORMAT (1H0,' YCO(SURFACE) =',/)
   43 FORMAT (1H0,' L/U =', F15.7/)
   44 FORMAT (1H0,' B1S, B2S, =', 4E15.8/)
   45 FORMAT (1H0,'B1, B2, B3, B4 =',4E15.8/)
   46 FORMAT (4E20.8)
   47 FORMAT (1H0,' E,S =',6F12.6/)
   48 FORMAT (1H0,'GC, XLEW1, XLEW2, XLS, DS =',6F12.6/)
   49 FORMAT (1H0,'RCI, XKI, CP, ALPHA =',3F12.6,E12.5/)
C
   71 FORMAT (1H0,'APPROACH VEL = ',F10.4/)
   72 FORMAT(1H0,'CHANNEL VEL (1.U.) = ',F10.5/)
   73 FORMAT (1H0,'EFFICIENCY(CARBON-BALANCE)',/)
   74 FORMAT (1H0,'EFFICIENCY(TEMPERATURE)',/)
  401 FORMAT (1H0,' XFI =', F20.5/)
  402 FORMAT (1H0,'TI, PR, REY, AD2UL, AOAS =',5F12.5/)
  403 FORMAT (1H0,' ES,S=',4E20.8/)
  404 FORMAT (1H0,'*******************************',/)
  405 FORMAT (1H0,'GAS TEMPERATURE IS NEGATIVE')
  406 FORMAT (1H0,' CNHM CONCENTRATION IS NEGATIVE')
  407 FORMAT (1H0,'  CO  CONCENTRATION IS NEGATIVE')
  408 FORMAT (1H0,' YFF IS NEGATIVE')
  409 FORMAT (1H0,'ADIABATIC FLAME TEMP =',F10.6/)
  410 FORMAT (1H0,'ADIAB FLAME TEMP(K) =',F15.5/)
C
C     ******************************************
C
C     ***********INPUT PARAMETERS*************
C
C     **********CHEMICAL PARAMETERS************
C
C
C     CHEMICAL REACTION 1,  CNHM + O2 = CO + H2O (GAS PHASE)
C     CHEMICAL REACTION 2, CO + O2 = CO2 (GAS PHASE)
C     CHEMICAL REACTION 3, CNHM + O2 = CO2 + H2O (SOLID SURFACE)
```

```
C       CHEMICAL REACTION 4, CO +O2 = CO2 (SOLID SURFACE)
C
C
C       ES1 = ACTIVATION ENERGY FOR REACTION 1 (CAL/MOLE),ETC.
C       C1 = PREEXPONENTIAL FACTOR (DIMENSIONAL) FOR REACTION 1, ETC.
C       WHC, WCO = MOLECULAR WEIGHTS FOR CNHM, CO
C       Q1S = HEAT OF COMBUSTION FOR REACTION 1 (CAL/G OF CNHM)
C       Q2S = HEAT OF COMBUSTION FOR REACTION 2 (CAL/G OF CO)
C       QS = HEAT OF COMBUSTION FOR REACTION 3 (CAL/G OF CNHM)
C
C       XN = THE NUMBER OF CARBONS IN CNHM
C       XM = THE NUMBER OF HYDROGEN IN CNHM
C
C
C
        QS = Q1S + Q2S*XN*WCO/WHC
C
C       ******** CATALYTIC BED PARAMETERS **************
C
C       XLS = BED LENGTH (M)
C       DS = CHANNEL HYDRAULIC DIAMETER (M)
C       SOA = CIRCUMFERENTIAL LENGTH DIVIDED BY CHANNEL AREA,=4/DS(1/M)
C       AOAS = RATIO OF OPEN TO CLOSED AREAS
C       CSS = HEAT CAPACITY OF SUBSTRATE (CAL/KG/K)
C       ROS = DENSITY OF SUBSTRATE (KG/M3)
C
C
        READ (5,10) XPHI
        READ (5,10) TI
        READ (5,10) XFI
        READ (5,10) UIUS
        READ (5,10) XLS
        READ (5,10) DS
        READ (5,10) AOAS
        READ (5,10) DX
        READ (5,10) DT
        READ (5,10) TMAX
        READ (5,8) IPRINT
        READ (5,8) N
        READ (5,8) NAS
        READ (5,*) C1,C2,C3,C4
        READ (5,8) IT
        SOA = 4.0/DS
        CN = XN*WCO/WHC
        NPNAS = N + NAS
C
C       ************** OPERATING PARAMETERS **************
C       TI = INITIAL, UPSTREAM (I.U.) TEMPERATURE (K)
C       UI = I.U. VELOCITY (M/S)
C       XPI = I.U. PRESSURE (ATM.)
C       ROI = I.U. GAS DENSITY (KG/M3)
C       YFI = I.U. MASS FRACTION OF HC
C       YCI = I.U. MASS FRACTION OF CO
C       YOI = I.U. MASS FRACTION OF O2
C       XPHI = UPSTREAM HC/O2 EQUIVALENCE RATIO
C
C
        UI = UIUS*(1.0+.OAS)/AOAS
        XMU = 0.000001458*SQRT(TI)/(1.0+110.4/TI)
        YFI = WHC*XPHI/29./((XN+XM/4.)*4.76+XPHI)
        XLEW1 = 1.5* SQRT (29./WHC)
        XLEW2 = 1.5* SQRT (29./WCO)
        XLE123=XLEW1**.667
        XLE223=XLEW2**.667
C
        XLOU = XLS/UI
C
C       *************** GAS PROPERTY ***************
C
C
C
C       CP = SPECIFIC HEAT OF GAS (CAL/KG/K)
C       XKI = HEAT CONDUCTIVITY OF GAS AT I.U. (CAL/M/SEC/K)
C       ALPHA = I.U. GAS THERMAL DIFFUSIVITY (M2/SEC)
C       GC=GAS CONSTANT FOR GAS MIXTURE (JOULE/KG/K)
C       XLEW1 = LEWIS NUMBER FOR CNHM IN MIXTURE
C       XLEW2 = LEWIS NUMBER FOR CO IN MIXTURE
C
C
        XKI=.003+.000013*TI
        ROI = XPI/GC/TI
        ALPHA = XKI/ROI/CP
```

```
16300           REY = UIUS*DS*RCI/XMU
16400     C
16500     C
16600     C     TO DESCRIBE CHEMICAL REACTION RATE EXPRESSIONS
16700     C     REACTION 1 (GAS PHASE)
16800     C     D(CNHM)/DT $$$ XP**.3*T*SQRT(YHC)*YO2/EXP(E1/RT)
16900     C
17000     C     REACTION 2 (GAS PHASE)
17100     C     D(CC)/DT $$$ YCC*SQRT(YO2)*SQRT(YH2O)/EXP(E2/RT)
17200     C
17300     C     REACTION 3 (SOLID SURFACE)
17400     C     D(CNHM)/DT $$$ YHCS/EXP(E3/RT)
17500     C
17600     C     REACTION 4 (SOLID SURFACE)
17700     C     D(CO)/DT $$$ YCCS/EXP(E4/RT)
17800     C
17900     C     TO EVALUATE KINETIC RATE CONSTANTS
18000     C
18100           B1SS = C1*SQRT(WHC)/WC2/SQRT(1000.)
18200           B1S = B1SS*XPI**.3*RCI*SQRT(RCI)*TI*SQRT(YFI)*YOI
18300           B1 = XLOU*B1S/RCI/YFI
18400           SSWO2=SQRT(SQRT(WO2))
18500     C
18600           B2SS = C2/1000.**.75/SSWO2/SQRT(WH2O)
18700           SSROI = SQRT(SQRT(ROI))
18800           SSYOI=SQRT(SQRT(YOI))
18900           B2S=B2SS*ROI*RCI/SSROI*YFI*SSYOI
19000           B2 = B2S*XLOU/RCI/YFI
19100     C
19200           B3 = C3*DS/ALPHA/WHC/3.66
19300           B4 = C4*DS/ALPHA/WCO/3.66
19400           Q1 = Q1S/CP/TI
19500           Q2 = Q2S/CP/TI
19600           Q = QS/CP/TI
19700           TAB = YFI*Q+1.0
19800           TABDM = TAB*TI
19900           E1 = ES1/TI/1.987
20000           E2 = ES2/TI/1.987
20100           E3 = ES3/TI/1.987
20200           E4 = ES4/TI/1.987
20300           AD2UL = (ALPHA/DS/DS)/(UI/XLS)
20400     C     ******************************
20500     C
20600           WRITE (6,21) N,NAS
20700           WRITE (6,20) TMAX
20800           WRITE (6,15) YCI, YFI, XPHI
20900           WRITE (6,71) UIUS
21000           WRITE (6,72) UI
21100           WRITE (6,17) Q1, Q2, DX, DT
21200           WRITE (6,402)TI,XPR,REY, AD2UL, AOAS
21300           WRITE (6,409) TAB
21400           WRITE (6,410) TABDM
21500           WRITE (6,403)ES1, ES2, ES3, ES4
21600           WRITE (6,47)E1, E2, E3, E4
21700           WRITE (6,35) C1, C2, C3, C4
21800           WRITE (6,48) GC, XLEW1, XLEW2, XLS, DS
21900           WRITE (6,49) RCI, XKI, CP, ALPHA
22000           WRITE (6,401) XPI
22100           WRITE (6,43) XLOU
22200           WRITE (6,44) B1S, B2S
22300           WRITE (6,45) B1, B2, B3, B4
22400           WRITE (6,19)
22500           WRITE (6,24) (TS (I), I=1,N,IT)
22600           WRITE (6,25)
22700           WRITE (6,24) (YFS(I), I=1,N,IT)
22800           WRITE (6,33)
22900           WRITE (6,24)(YCS(I), I=1,N,IT)
23000     C
23100     C     ******************************
23200     C
23300     C     ************ UPSTREAM CONDITIONS ************
23400           YF(1) = 1.
23500           YC(1) = 0.0
23600           YO(1) = 1.
23700           T(1) = 1.
23800           RO(1) = 1.
23900           XP(1) = 1.0
24000           U(1) = 1.
24100     C
24200     C     ***********************************************
24300     C
```

```
24400    C      ********************************************
24500    C      START OF INTEGRATION LOOP
24600           KOUNT = 1
24700           XNU0 = .885*SQRT(AOAS)*SQRT(XPR*RFY)
24800           ROOT1 = 0.0
24900           ROOT2 = 1.0
24950      555  CONTINUE
25000           ROOT = .5*(ROOT1 + ROOT2)
25100           IF(ROOT.LE.0.1)YNU=.0444/ROOT+3.46-1.34*ROOT
25200           IF(ROOT.GT.0.1)YNU=0.011/ROOT+3.66
25300           YROOT=YNU-XNU0
25400           IF (ABS(YROOT).LT.0.01) GO TO 200
25500           IF (YROOT.GT.0.0) ROOT1=ROOT
25600           IF (YROOT.LE.0.0) ROOT2=ROOT
25700           GO TO 555
25800      200  CONTINUE
25900           DMASS=RO(1)*U(1)
26000    C
26100    C      INTEGRATION OF QUASI-STEADY GAS PHASE EQUATIONS FOR
26200    C      YF (FUEL MASS FRACTION) AND T (TEMPERATURE) IN DOWNSTREAM
26300    C      DIRECTION USING FOURTH-ORDER RUNGE-KUTTA SCHEME
26400    C      I IS THE INDEX FOR DOWNSTREAM DISTANCE X
26500    C
26600    C
26700           DO 201 I=1, NPNAS
26800    C
26900           IF(I.GT.N)DMASS=RO(1)*U(1)*ACAS/(ACAS+1.)
27000    C      ********************************************
27100    C
27200    C      EVALUATE XJH AND XJD AS A FUNCTION OF X
27300    C
27400    C      ********************************************
27500    C      NONDIMENSIONAL HEAT CONDUCTIVITY
27600           XK = (.003 + 0.000013* TI *T(I))/XK1
27700    C      ********************************************
27800    C
27900           IF(I.GT.1) GO TO 180
28000           IF(I.EQ.1) X=0.0
28100           GO TO 181
28150      180  CONTINUE
28300           IX=I+1
28400           XI=IX-1
28500           X = XI*DX
28600      181  CONTINUE
28700           XST = X*2.0*AD2UL*XK+ROOT
28800           IF (XST.LE.0.1) XNU=0.0444/XST+3.46-1.34*XST
28900           IF (XST.GT.0.1) XNU=0.011/XST +3.66
29000           RNK(I)=XNU*XK/3.66
29100           XJH(I) = 4.0*XNU *AD2UL*XK
29200           IF (I.GT.N) XJH(I) = 0.0
29300           XJD1(I) = XJH(I) *XLE123
29400           XJD2(I) = XJH(I) *XLE223
29500    C      ********************************************
29600    C
29700      132  CONTINUE
29800           M=1
29900           DO 120 L=1,4
30000           IF (M.NE.1) GO TO 102
30100           YFF = YF(I)
30200           YCC = YC(I)
30300           TT = T(I)
30400           M = M+1
30500           GO TO 119
30600      102  CONTINUE
30700           IF (M.NE.2) GO TO 103
30800           YFF=YF(I)+DX*XKY(1)/2.
30900           YCC = YC(I) +DX*XKC(1)/2.
31000           TT=T(I)+XKT(1)*DX/2.
31100           M=M+1
31200           GO TO 119
31300      103  CONTINUE
31400           IF(M.NE.3) GO TO 104
31500           YFF = YF(I) + DX*XKY(2)/2.
31600           YCC = YC(I) + DX*XKC(2)/2.
31700           TT=T(I)+DX*XKT(2)/2.
31800           M=M+1
31900           GO TO 119
32000      104  CONTINUE
32100           YFF = YF(I) + DX*XKY(3)
32200           YCC = YC(I) + DX*XKC(3)
32300           TT=T(I) +DX*XKT(3)
```

```
32400      119 CONTINUE
32500    C     YH2C = MASS FRACTION OF H2O
32600          YH2C(I) = .5*XM*WH2O*YFI* (YF(1)-YF(I))/WHC
32650          IF(YFF.LT.0.0) YFF=0.0
32700          W1 = B1* XP(I)**.3*RC(I)*SQRT(RO(I))*T(I)*SQRT(YFF)*YO(I)
32800         1/EXP(E1/TT)
32900          SSYC=SQRT(SQRT(YO(I)))
33000          RO175=RO(I)*RG(I)/SQRT(SQRT(RC(I)))
33100          W2=B2*RO175*YCC*SSYC*SQRT(YH2C(I))/EXP(E2/TI)
33200          XKY(L) = -XJD1(I) *(YFF- YFS(I))/DMASS -W1/DMASS
33300          XKC(L) = -XJD2(I) *(YCC-YCS(I))/ DMASS +CN*W1/DMASS -W2/DMASS
33400          XKT(L) =-XJH(I)*(TT-TS(I))/DMASS+Q1*YFI*W1/DMASS+Q2*YFI*W2/DMASS
33500      120 CONTINUE
33600          YF(I+1) =YF(I) +DX*(XKY (1)/6. +XKY (2)/3. +XKY (3)/3.+XKY (4)/6.)
33700          IF (YF(I+1).LT.0.0) YF(I+1) =0.0
33800          YC(I+1)=YC(I)+DX*(XKC(1)/6.+XKC(2)/3.+XKC(3)/3.+XKC(4)/6.)
33900          IF (YC(I+1).LT.0.0) YC(I+1) =0.0
34000          T (I+1) =T (I) +DX*(XKT (1)/6. +XKT (2)/3. +XKT (3)/3.+XKT (4)/6.)
34100          IF (T(I+1).LT.0.0) GO TO 601
34200          ADD=YC(I+1)*YFI*WO2/YCI/WCO/2.
34300          YO(I+1) =1.0-XPHI*(1.0-YF(I+1))+ADD
34400          XP(I+1)=XP(I)
34500          RO(I+1)=XP(I+1) /T(I+1)
34600          U(I+1) =DMASS/T(I+1)
34700          EFF(I)=1.-YF(I)-YC(I)*Q2/Q
34800          EFFT(I)=(T(I)-T(1))/(TAB-T(1))
34900      201 CONTINUE
35000    C
35100    C     END OF ONE RUNGE-KUTTA INTEGRATION CYCLE FOR QUASI-STEADY
35200    C     GAS PHASE EQUATIONS
35300    C     ***************************************************************
35400    C
35500    C
35600    C     ***************************************************************
35700    C     INTEGRATION OF UNSTEADY SOLID HEAT TRANSFER EQUATION
35800    C     FOR TS (SOLID TEMPERATURE) IN TIME USING FOURTH-ORDER
35900    C     RUNGE-KUTTA SCHEME
36000    C
36100    C
36200    C
36300          DO 301 J =1,N
36400          MJ=1
36500          DO 320 LJ=1,4
36600          IF (MJ.NE.1) GO TO 302
36700          TSS =TS(J)
36800          MJ=MJ+1
36900          GO TO 319
37000      302 CONTINUE
37100          IF(MJ.NE.2) GO TO 303
37200          TSS = TS(J) + DT*XKTS(1)/2.
37300          MJ=MJ+1
37400          GO TO 319
37500      303 CONTINUE
37600          IF(MJ.NE.3) GO TO 304
37700          TSS=TS(J)+DT*XKTS(2) /2.
37800          MJ=MJ+1
37900          GO TO 319
38000      304 CONTINUE
38100          TSS = TS(J) + DT* XKTS(3)
38200      319 CONTINUE
38300          XKTS(LJ)=RNK(J)*(T(J)-TSS) +B3*YFI*Q*RO(J)*YFS(J)/EXP(E3/TSS)
38400         1 +B4*YFI*Q2*RO(J)*YCS(J)/EXP(E4/TSS)
38500      320 CONTINUE
38600          TS(J) =TS(J) +DT*(XKTS(1)/6.+XKTS(2)/3.+XKTS(3)/3.+XKTS(4)/6.)
38700          YFS(J) = YF(J) /(1.+B3*RO(J)/XLE123/RNK(J)/EXP(E3/TS(J)))
38800          YCS(J) = YC(J) /(1.+B4*RO(J)/XLE223/RNK(J)/EXP(E4/TS(J)))
38900      301 CONTINUE
39000    C
39100    C     END OF ONE TIME INTEGRATION STEP
39200    C     ***************************************************************
39300    C
39400    C     ***************************************************************
39500    C     LOOP FOR MARCHING FORWARD IN TIME
39600    C
39700          KOUNT = KOUNT+1
39800          KOU   = KOUNT-1
39900          XKOUNT = KOUNT
40000          TIME=(XKOUNT-1.)*DT
40100          IF (TIME.GT. TMAX) GO TO 999
40200          IF (MOD(KOU,IPRINT).NE.0) GO TO 200
```

```
40300           WRITE(6,22) TIME  ,KOUNT
40400           WRITE (6,13)
40500           WRITE(6,24) (T  (I),I=1,NPNAS,IT)
40600           WRITE (6,9)
40700           WRITE(6,24) (TS (I), I=1,N,IT)
40800           WRITE(6,14)
40900           WRITE(6,24)  (YF(I),I=1,NPNAS,IT)
41000           WRITE(6,41)
41100           WRITE(6,24)  (YC(I),I=1,NPNAS,IT)
41200           WRITE(6,11)
41300           WRITE(6,24)  (YFS(I),I=1,N,IT)
41400           WRITE(6,42)
41500           WRITE(6,24)  (YCS(I),I=1,N,IT)
41600           WRITE(6,26)
41700           WRITE(6,24) (XJH(I),I=1,N,IT)
41800           WRITE(6,73)
41900           WRITE(6,24)  (EFF(I),I=1,NPNAS,IT)
42000           WRITE(6,74)
42100           WRITE(6,24)  (EFFT(I),I=1,NPNAS,IT)
42200           WRITE(6,23)
42300           GO TO 200
42400     C
42500     C     END OF WHOLE INTEGRATION LOOP
42600     C     ************************************************************
42700     C
42800       601 CONTINUE
42900           WRITE (6,404)
43000           WRITE(6,405)
43100       999 CONTINUE
43200           STOP
43300           END
```

```
  100         BLOCK DATA
  200
  300         DIMENSION TS(300),YFS(300),YCS(300)
  400         COMMON /ACTI/ES1,ES2,ES3,ES4
  600         COMMON /MOLEQ/ WHC, WCO, WO2, WH2O
  700         COMMON /TH1/XN, XM, Q1S, Q2S
  800         COMMON /TH2/ CP, GC,  XPR
  900         COMMON /UPST/ YCI, YOI
 1100         COMMON /INI/TS,YFS,YCS
 1200
 1400         DATA ES1,ES2,ES3,ES4/24000.,40000.,10000.,17000./
 1500         DATA WHC,WCO,WO2,WH2O/44.,28.,32.,18./
 1600         DATA XN,XM,Q1S,Q2S/3.,8.,6491000.,2415000./
 1700         DATA CP,GC,XPR/265.,2.8312E-3,0.7/
 1800         DATA YCI,YOI/0.,0.23/
 2000         DATA TS,YFS,YCS/300*1.,300*0.,300*0./
 2100         END
```

Example calculation:

```
$ RUN IGNITION.EXE;10
.18
1000.
3.
10.
.1
.0016
2.
.01
.01
1.001
  20
  46
  80
1.5E5 0.71E14 2.5E3 1.E5
   5
```

read-in data:
- ϕ
- TI
- XPI
- UIUS
- XLS
- DS
- AOAS
- DX
- DT
- TMAX
- IPRINT
- N
- NAS
- C1, C2, C3, C4
- IT

```
NO. OF GRID POINT =         46         80


TMAX =       1.00100005

YO(UPST,INI) =   0.230000      YF(UPST,INI)= 0.0113888      EQUI RATIO =     0.18000
0007


APPROACH VEL =     10.0000

CHANNEL VEL (I.U.) =    15.00000
```

```
01=      22.7754402      02=       8.4736843      DX=       0.0100000      DT=       0.
0100000


TI, PR, REY, AD2UL, ADAS =  1000.00000      0.70000   408.31238      0.13797      2
.00000

ADIABATIC FLAME TEMP =  1.443622

ADIAB FLAME TEMP(K) =      1443.62195

 ES,S=       0.24000000E+05       0.40000000E+05       0.10000000E+05       0.178000
00E+05

 E,S =    12.078510    20.130850     5.032712     8.958228

  C,S =       0.1500000000E+06     0.7100000371E+14     0.2500000000E+04     0.100000
0000E+06

GC, XLEW1, XLEW2, XLS, DS =     0.002831     1.217766     1.526551     0.100000     0
.001600

ROI, XKI, CP, ALPHA =     1.059621     0.016000  285.000000 0.52982E-04

 XPI =              3.00000

 L/U =       0.0066667

 B1S, B2S, = 0.36601332E+05 0.34534906E+09

B1, B2, B3, B4 = 0.20219805E+05 0.19078240E+09 0.46881531E+03 0.29468391E+05


INITIAL CONDITIONS (TS)

0.10000E+01 0.10000E+01 0.10000E+01 0.10000E+01 0.10000E+01 0.10000E+01 0.10000E
+01 0.10000E+01 0.10000E+01 0.10000E+01

INITIAL CONDITIONS (YFS)

0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00

INITIAL CONDITIONS (YCS)

0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
```

```
TIME=      0.20000000      KOUNT=          21


GAS TEMPERATURE (T)

0.10000E+01 0.10279E+01 0.10351E+01 0.10393E+01 0.10420E+01 0.10437E+01 0.10447E
+01 0.10451E+01 0.10451E+01 0.10447E+01
0.10462E+01 0.10481E+01 0.10501E+01 0.10521E+01 0.10541E+01 0.10562E+01 0.10583E
+01 0.10604E+01 0.10625E+01 0.10647E+01
0.10669E+01 0.10691E+01 0.10714E+01 0.10737E+01 0.10760E+01 0.10784E+01

SOLID TEMPERATURE (TS)

0.11390E+01 0.10786E+01 0.10631E+01 0.10542E+01 0.10477E+01 0.10427E+01 0.10384E
+01 0.10349E+01 0.10321E+01 0.10295E+01

CNHM MASS FRACTION (YF)

0.10000E+01 0.82811E+00 0.72848E+00 0.64850E+00 0.58054E+00 0.52141E+00 0.46932E
+00 0.42307E+00 0.38150E+00 0.34400E+00
0.33115E+00 0.32383E+00 0.31646E+00 0.30902E+00 0.30153E+00 0.29398E+00 0.28638E
+00 0.27871E+00 0.27100E+00 0.26324E+00
0.25542E+00 0.24756E+00 0.23966E+00 0.23171E+00 0.22373E+00 0.21571E+00

 YCO =

0.00000E+00 0.11484E-01 0.22136E-01 0.31487E-01 0.39522E-01 0.46303E-01 0.51923E
-01 0.56483E-01 0.60031E-01 0.62661E-01
0.73834E-01 0.87281E-01 0.10073E+00 0.11418E+00 0.12762E+00 0.14103E+00 0.15440E
+00 0.16772E+00 0.18098E+00 0.19417E+00
0.20726E+00 0.22024E+00 0.23309E+00 0.24579E+00 0.25833E+00 0.27068E+00

SURFACE HC MASS FRACTION (YFS)

0.53851E+00 0.24678E+00 0.20088E+00 0.17326E+00 0.15271E+00 0.13598E+00 0.12175E
+00 0.10985E+00 0.99795E-01 0.90590E-01

 YCO(SURFACE) =

0.00000E+00 0.26429E-02 0.48789E-02 0.68753E-02 0.86412E-02 0.10176E-01 0.11484E
-01 0.12628E-01 0.13636E-01 0.14440E-01

XJH

0.11677E+02 0.32271E+01 0.26856E+01 0.24599E+01 0.23328E+01 0.22489E+01 0.21875E
+01 0.21536E+01 0.21464E+01 0.21403E+01

EFFICIENCY(CARBON-BALANCE)

0.00000E+00 0.16939E+00 0.26670E+00 0.34465E+00 0.41086E+00 0.46852E+00 0.51939E
+00 0.56464E+00 0.60544E+00 0.64237E+00
0.65279E+00 0.65718E+00 0.66163E+00 0.66614E+00 0.67071E+00 0.67534E+00 0.68004E
+00 0.68480E+00 0.68963E+00 0.69452E+00
0.69949E+00 0.70453E+00 0.70964E+00 0.71482E+00 0.72008E+00 0.72541E+00

EFFICIENCY(TEMPERATURE)

0.00000E+00 0.62838E-01 0.79086E-01 0.88607E-01 0.94669E-01 0.98477E-01 0.10066E
+00 0.10160E+00 0.10161E+00 0.10085E+00
0.10409E+00 0.10848E+00 0.11292E+00 0.11743E+00 0.12200E+00 0.12663E+00 0.13133E
+00 0.13609E+00 0.14092E+00 0.14582E+00
0.15079E+00 0.15582E+00 0.16093E+00 0.16611E+00 0.17137E+00 0.17670E+00
```

```
TIME=      0.40000001      KOUNT=          41

GAS TEMPERATURE (T)

0.10000E+01 0.10491E+01 0.10635E+01 0.10720E+01 0.10776E+01 0.10811E+01 0.10833E
+01 0.10843E+01 0.10845E+01 0.10841E+01
0.10861E+01 0.10889E+01 0.10917E+01 0.10945E+01 0.10975E+01 0.11004E+01 0.11035E
+01 0.11065E+01 0.11097E+01 0.11129E+01
0.11161E+01 0.11194E+01 0.11228E+01 0.11262E+01 0.11297E+01 0.11332E+01

SOLID TEMPERATURE (TS)

0.12213E+01 0.11518E+01 0.11246E+01 0.11083E+01 0.10964E+01 0.10869E+01 0.10789E
+01 0.10722E+01 0.10667E+01 0.10617E+01

CNHM MASS FRACTION (YF)

0.10000E+01 0.80758E+00 0.70137E+00 0.61707E+00 0.54601E+00 0.48467E+00 0.43108E
+00 0.38389E+00 0.34185E+00 0.30433E+00
0.28925E+00 0.27908E+00 0.26883E+00 0.25851E+00 0.24813E+00 0.23769E+00 0.22719E
+00 0.21666E+00 0.20609E+00 0.19550E+00
0.18489E+00 0.17429E+00 0.16370E+00 0.15314E+00 0.14264E+00 0.13221E+00

 YCO =

0.00000E+00 0.13222E-01 0.26772E-01 0.39234E-01 0.50220E-01 0.59608E-01 0.67399E
-01 0.73657E-01 0.78404E-01 0.81781E-01
0.96870E-01 0.11495E+00 0.13288E+00 0.15060E+00 0.16809E+00 0.18529E+00 0.20218E
+00 0.21869E+00 0.23479E+00 0.25040E+00
0.26548E+00 0.27995E+00 0.29376E+00 0.30682E+00 0.31907E+00 0.33043E+00

SURFACE HC MASS FRACTION (YFS)

0.46424E+00 0.19836E+00 0.16474E+00 0.14380E+00 0.12762E+00 0.11403E+00 0.10218E
+00 0.92277E-01 0.83510E-01 0.75424E-01

 YCO(SURFACE) =

0.00000E+00 0.20352E-02 0.42042E-02 0.63776E-02 0.84571E-02 0.10376E-01 0.12090E
-01 0.13661E-01 0.15024E-01 0.16140E-01

XJH

0.11677E+02 0.32624E+01 0.27297E+01 0.25095E+01 0.23858E+01 0.23039E+01 0.22435E
+01 0.22180E+01 0.22112E+01 0.22049E+01

EFFICIENCY(CARBON-BALANCE)

0.00000E+00 0.18954E+00 0.29281E+00 0.37440E+00 0.44306E+00 0.50236E+00 0.55425E
+00 0.60008E+00 0.64109E+00 0.67788E+00
0.68968E+00 0.69592E+00 0.70227E+00 0.70873E+00 0.71531E+00 0.72200E+00 0.72882E
+00 0.73577E+00 0.74284E+00 0.75003E+00
0.75736E+00 0.76481E+00 0.77240E+00 0.78011E+00 0.78795E+00 0.79591E+00

EFFICIENCY(TEMPERATURE)

0.00000E+00 0.11074E+00 0.14304E+00 0.16233E+00 0.17485E+00 0.18292E+00 0.18775E
+00 0.19010E+00 0.19058E+00 0.18953E+00
0.19407E+00 0.20031E+00 0.20666E+00 0.21312E+00 0.21970E+00 0.22640E+00 0.23322E
+00 0.24016E+00 0.24723E+00 0.25443E+00
0.26175E+00 0.26921E+00 0.27679E+00 0.28451E+00 0.29234E+00 0.30031E+00
```

```
TIME=      0.59999996      KOUNT=          61

GAS TEMPERATURE (T)

0.10000E+01 0.10637E+01 0.10848E+01 0.10979E+01 0.11067E+01 0.11127E+01 0.11166E
+01 0.11188E+01 0.11198E+01 0.11197E+01
0.11225E+01 0.11262E+01 0.11301E+01 0.11340E+01 0.11380E+01 0.11421E+01 0.11463E
+01 0.11506E+01 0.11550E+01 0.11594E+01
0.11640E+01 0.11686E+01 0.11733E+01 0.11780E+01 0.11828E+01 0.11876E+01

SOLID TEMPERATURE (TS)

0.12635E+01 0.12134E+01 0.11791E+01 0.11578E+01 0.11419E+01 0.11289E+01 0.11179E
+01 0.11088E+01 0.11011E+01 0.10940E+01

CNHM MASS FRACTION (YF)

0.10000E+01 0.79629E+00 0.68495E+00 0.59669E+00 0.52239E+00 0.45843E+00 0.40278E
+00 0.35401E+00 0.31086E+00 0.27270E+00
0.25498E+00 0.24161E+00 0.22817E+00 0.21469E+00 0.20118E+00 0.18767E+00 0.17418E
+00 0.16074E+00 0.14739E+00 0.13416E+00
0.12109E+00 0.10825E+00 0.95689E-01 0.83472E-01 0.71677E-01 0.60388E-01

 YCO =

0.00000E+00 0.14469E-01 0.30578E-01 0.46066E-01 0.60086E-01 0.72238E-01 0.82367E
-01 0.90438E-01 0.96435E-01 0.10054E+00
0.11961E+00 0.14221E+00 0.16422E+00 0.18553E+00 0.20602E+00 0.22560E+00 0.24413E
+00 0.26148E+00 0.27750E+00 0.29206E+00
0.30499E+00 0.31614E+00 0.32534E+00 0.33244E+00 0.33728E+00 0.33972E+00

SURFACE HC MASS FRACTION (YFS)

0.43022E+00 0.16752E+00 0.14035E+00 0.12323E+00 0.10966E+00 0.97974E-01 0.87588E
-01 0.78891E-01 0.70921E-01 0.63536E-01

 YCO(SURFACE) =

0.00000E+00 0.16102E-02 0.35915E-02 0.57604E-02 0.79705E-02 0.10111E-01 0.12099E
-01 0.13980E-01 0.15616E-01 0.16983E-01

XJH

0.11677E+02 0.32865E+01 0.27628E+01 0.25486E+01 0.24291E+01 0.23501E+01 0.22915E
+01 0.22746E+01 0.22690E+01 0.22633E+01

EFFICIENCY(CARBON-BALANCE)

0.00000E+00 0.20056E+00 0.30840E+00 0.39329E+00 0.46453E+00 0.52586E+00 0.57930E
+00 0.62632E+00 0.66817E+00 0.70543E+00
0.71900E+00 0.72746E+00 0.73610E+00 0.74495E+00 0.75400E+00 0.76325E+00 0.77271E
+00 0.78238E+00 0.79225E+00 0.80231E+00
0.81256E+00 0.82298E+00 0.83354E+00 0.84421E+00 0.85495E+00 0.86571E+00

EFFICIENCY(TEMPERATURE)

0.00000E+00 0.14356E+00 0.19111E+00 0.22064E+00 0.24056E+00 0.25404E+00 0.26275E
+00 0.26777E+00 0.26994E+00 0.26975E+00
0.27609E+00 0.28455E+00 0.29320E+00 0.30204E+00 0.31109E+00 0.32034E+00 0.32980E
+00 0.33947E+00 0.34934E+00 0.35940E+00
0.36965E+00 0.38007E+00 0.39063E+00 0.40130E+00 0.41204E+00 0.42280E+00
```

TIME= 0.80000001 KOUNT= 81

GAS TEMPERATURE (T)

0.10000E+01 0.10736E+01 0.11008E+01 0.11183E+01 0.11306E+01 0.11392E+01 0.11452E
+01 0.11490E+01 0.11512E+01 0.11519E+01
0.11557E+01 0.11606E+01 0.11656E+01 0.11708E+01 0.11761E+01 0.11816E+01 0.11871E
+01 0.11928E+01 0.11986E+01 0.12045E+01
0.12104E+01 0.12162E+01 0.12220E+01 0.12276E+01 0.12330E+01 0.12380E+01

SOLID TEMPERATURE (TS)

0.12842E+01 0.12637E+01 0.12263E+01 0.12021E+01 0.11836E+01 0.11683E+01 0.11551E
+01 0.11442E+01 0.11347E+01 0.11258E+01

CNHM MASS FRACTION (YF)

0.10000E+01 0.78985E+00 0.67457E+00 0.58286E+00 0.50547E+00 0.43878E+00 0.38082E
+00 0.33013E+00 0.28551E+00 0.24636E+00
0.22574E+00 0.20896E+00 0.19220E+00 0.17549E+00 0.15888E+00 0.14244E+00 0.12625E
+00 0.11038E+00 0.94950E-01 0.80069E-01
0.65879E-01 0.52539E-01 0.40228E-01 0.29146E-01 0.19511E-01 0.11553E-01

YCO =

0.00000E+00 0.15324E-01 0.33574E-01 0.51842E-01 0.68808E-01 0.83726E-01 0.96218E
-01 0.10609E+00 0.11328E+00 0.11798E+00
0.14070E+00 0.16711E+00 0.19204E+00 0.21529E+00 0.23659E+00 0.25571E+00 0.27238E
+00 0.28632E+00 0.29728E+00 0.30498E+00
0.30918E+00 0.30970E+00 0.30638E+00 0.29913E+00 0.28799E+00 0.27306E+00

SURFACE HC MASS FRACTION (YFS)

0.41453E+00 0.14723E+00 0.12338E+00 0.10845E+00 0.96428E-01 0.85904E-01 0.76418E
-01 0.68448E-01 0.60959E-01 0.54005E-01

YCO(SURFACE) =

0.00000E+00 0.13253E-02 0.30987E-02 0.51695E-02 0.73836E-02 0.96090E-02 0.11737E
-01 0.13799E-01 0.15599E-01 0.17119E-01

XJH

0.11677E+02 0.33030E+01 0.27876E+01 0.25795E+01 0.24646E+01 0.23889E+01 0.23328E
+01 0.23243E+01 0.23206E+01 0.23162E+01

EFFICIENCY(CARBON-BALANCE)

0.00000E+00 0.20682E+00 0.31813E+00 0.40586E+00 0.47956E+00 0.54301E+00 0.59825E
+00 0.64679E+00 0.68985E+00 0.72798E+00
0.74366E+00 0.75469E+00 0.76603E+00 0.77768E+00 0.78965E+00 0.80193E+00 0.81450E
+00 0.82733E+00 0.84038E+00 0.85359E+00
0.86686E+00 0.88009E+00 0.89312E+00 0.90578E+00 0.91784E+00 0.92905E+00

EFFICIENCY(TEMPERATURE)

0.00000E+00 0.16600E+00 0.22721E+00 0.26670E+00 0.29434E+00 0.31389E+00 0.32731E
+00 0.33593E+00 0.34078E+00 0.34242E+00
0.35100E+00 0.36203E+00 0.37337E+00 0.38503E+00 0.39700E+00 0.40928E+00 0.42185E
+00 0.43468E+00 0.44773E+00 0.46093E+00
0.47421E+00 0.48744E+00 0.50047E+00 0.51313E+00 0.52519E+00 0.53639E+00

```
TIME=      1.00000000      KOUNT=         101

GAS TEMPERATURE (T)

0.10000E+01 0.10805E+01 0.11129E+01 0.11345E+01 0.11501E+01 0.11616E+01 0.11698E
+01 0.11755E+01 0.11792E+01 0.11811E+01
0.11861E+01 0.11922E+01 0.11986E+01 0.12052E+01 0.12120E+01 0.12189E+01 0.12259E
+01 0.12330E+01 0.12401E+01 0.12470E+01
0.12536E+01 0.12597E+01 0.12651E+01 0.12696E+01 0.12730E+01 0.12757E+01

SOLID TEMPERATURE (TS)

0.12942E+01 0.13041E+01 0.12666E+01 0.12412E+01 0.12213E+01 0.12045E+01 0.11899E
+01 0.11778E+01 0.11670E+01 0.11568E+01

CNHM MASS FRACTION (YF)

0.10000E+01 0.78602E+00 0.66774E+00 0.57313E+00 0.49291E+00 0.42358E+00 0.36325E
+00 0.31050E+00 0.26422E+00 0.22386E+00
0.20022E+00 0.18001E+00 0.15997E+00 0.14021E+00 0.12085E+00 0.10205E+00 0.83997E
-01 0.66901E-01 0.51025E-01 0.36667E-01
0.24163E-01 0.13877E-01 0.61870E-02 0.14578E-02 0.00000E+00 0.00000E+00

 YCO =

0.00000E+00 0.15904E-01 0.35886E-01 0.56611E-01 0.76315E-01 0.93878E-01 0.10864E
+00 0.12020E+00 0.12840E+00 0.13347E+00
0.15912E+00 0.18804E+00 0.21403E+00 0.23668E+00 0.25556E+00 0.27025E+00 0.28033E
+00 0.28546E+00 0.28534E+00 0.27984E+00
0.26894E+00 0.25285E+00 0.23195E+00 0.20684E+00 0.17831E+00 0.15073E+00

SURFACE HC MASS FRACTION (YFS)

0.40722E+00 0.13348E+00 0.11127E+00 0.97579E-01 0.86488E-01 0.76671E-01 0.67731E
-01 0.60191E-01 0.52984E-01 0.46285E-01

 YCO(SURFACE) =

0.00000E+00 0.11340E-02 0.27210E-02 0.46606E-02 0.68086E-02 0.90267E-02 0.11191E
-01 0.13321E-01 0.15180E-01 0.16751E-01

XJH

0.11677E+02 0.33143E+01 0.28063E+01 0.26039E+01 0.24936E+01 0.24215E+01 0.23683E
+01 0.23678E+01 0.23657E+01 0.23641E+01

EFFICIENCY(CARBON-BALANCE)

0.00000E+00 0.21052E+00 0.32445E+00 0.41456E+00 0.49049E+00 0.55600E+00 0.61311E
+00 0.66335E+00 0.70785E+00 0.74710E+00
0.76517E+00 0.77909E+00 0.79347E+00 0.80830E+00 0.82355E+00 0.83916E+00 0.85502E
+00 0.87100E+00 0.88690E+00 0.90246E+00
0.91733E+00 0.93112E+00 0.94335E+00 0.95355E+00 0.96121E+00 0.96721E+00

EFFICIENCY(TEMPERATURE)

0.00000E+00 0.18145E+00 0.25441E+00 0.30314E+00 0.33837E+00 0.36422E+00 0.38283E
+00 0.39570E+00 0.40395E+00 0.40818E+00
0.41940E+00 0.43332E+00 0.44770E+00 0.46253E+00 0.47778E+00 0.49339E+00 0.50925E
+00 0.52523E+00 0.54113E+00 0.55669E+00
0.57156E+00 0.58535E+00 0.59758E+00 0.60778E+00 0.61546E+00 0.62146E+00
```

APPENDIX II

LISTING OF COMPUTER PROGRAMS FOR CHAPTER II

The computer programs for Part II (steady state) are quite similar, in structure, to those in Part I. In addition to using a three-reactions scheme as discussed in the text of Part II, only the final results are printed out (no intermediate transient).

More Detailed Instruction (for CALY1. FOR; 75):

1. Read-in data (lines 10400 - 11475):

   XPHI = ϕ = fuel-air equivalence ratio

   TI = T(0,0) = upstream, initial temperature (K)

   XPI = p(0,0) = upstream, initial pressure (Atm.)

   UIUS = U_{ref} = upstream (outside of the bed) initial gas velocity (m/s)

   XLS = reference length (m), suggested to use 0.1m (10 cm)

   DS = d* = channel hydraulic diameter (m)

   AOAS = A^*/A_s^* = open-to-close area ratio

   DXX = nondimensional step size in X (space) inside the catalytic bed. It is nondimensionalized by XLS. So if XLS = 0.1 m and DX = 0.01, the dimensional step size is 0.001 m or 1mm.

   XAS = ratio of step sizes between downstream and inside-bed regions. For example, (XAS) x (DXX) is the integration step size in X - direction in the downstream space.

   DT = nondimensional time step size, recommended to be 0.2 or 0.1 for steady calculations.

   TMAX = maximum nondimensional time allowed for computation. It should be large enough to allow the steady state to be reached. For bed length less than 5 cm, TMAX = 8.001 is suggested, for bed length between 5 - 12 cm, TMAX = 12.001 is suggested.

N = number of grid points (in X direction) in the catalytic bed. The nondimensional catalytic bed length is given by (N-1) x (DX). For example, if N = 51, DX = .01, then the nondimensional bed length is equal to 0.5. If XLS = .1m, then the dimensional bed length is .05m (5 cm).

NAS = number of grid points (in X - direction) in the downstream after-bed space. The length of the downstream distance can be calculated in a similar manner as in the above.

IT = interval in X for printout. For example, if DXX =.01, IT = 5, the printout will be at X = 0, 0.05, 0.1, 0.15, etc. ...

CO, C1, C2, C3, C4 = C_1, C_2, C_3, C_4 (See Table I)

IPUTIN = 1 (always)

2. Output data (lines 37000 -38586):

The following quantities will be printed out as a function of downstream distance:

Gas and solid temperatures, Emission indices (x1000) for the original hydrocarbon, pyrolyzed hydrocarbon, total hydrocarbon and CO in the gas phase, the original hydrocarbon and CO at the wall and the combustion efficiency.

If TMAX is large enough, the above printouts are the steady-state profiles.

```
C
C     ***************************************
C     ***   STEADY  CATALYTIC COMBUSTION ***
C     ***************************************
C
C     THREE GAS-PHASE REACTION STEPS
C
C     VARIABLE X STEP SIZE ( BED VS. AFTER-BED SPACE )
C
      PARAMETER NX=300
      COMMON /ACTI/ ES0,ES1,ES2,ES3,ES4
      COMMON /MOLEQ/ WHC, WCC, WO2, WH2O
      COMMON /TH1/XN, XM, Q1S, Q2S
      COMMON /TH2/ CP, GC,  XPR
      COMMON /UPST/ YCI, YOI
      COMMON /INI/TS,YFS,YCS,YES
      COMMON /B12345/BTA1,BTA2,BTA3,BTA4,BTA5
      COMMON /GAMMA/GAMA
C
      DIMENSION YF(NX), T(NX), TS(NX), YO(NX), YFS(NX) ,HC(NX), U(NX)
      DIMENSION XKY(4), XKT(4), XKTS(4),XKC(4), YC(NX), YCS(NX)
      DIMENSION  XJH(NX), XJD1(NX), XJD2(NX) , YH2O(NX)  ,XP(NX)
      DIMENSION EFF(NX), RNK(NX)
      DIMENSION A(NX,3), XKE(4),YE(NX),YTHC(NX),YES(NX)
      EQUIVALENCE (A(1,1),TS(1)), (A(1,2),YFS(1)), (A(1,3),YCS(1))
C
    7 FORMAT (4E20.10)
    8 FORMAT (I4)
    9 FORMAT (1H0,'SOLID TEMPERATURE (TS)'/)
   10 FORMAT (6F12.6)
   11 FORMAT (1H0,'SURFACE  HC  MASS FRACTION (YFS)'/)
   12 FORMAT (//)
   13 FORMAT (1H0,'GAS TEMPERATURE (T)'/)
   14 FORMAT(1H0,'ORIGINAL CNHM (YF)'/)
   15 FORMAT(1H0,'YO(UPST,INI) =', F10.6,5X, 'YF (UPST,INI) =',F10.7,
     1   5X,'EQUI RATIO =', F15.9//)
   17 FORMAT (1H0,'Q1=',F15.7,5X,'Q2=', F15.7,5X,'DX=',F15.7,5X,'DT=',
     1F15.7//)
   18 FORMAT (1H0,'N=',I10//)
   19 FORMAT (1H0,'INITIAL CONDITIONS (TS)',/)
   20   FORMAT (1H0,'TMAX = ',F15.8)
   21 FORMAT (1H0,'NO. OF GRID POINT =',2I10//)
   22 FORMAT (1H0,'TIME=',F15.8,5X,'KOUNT=',I10/)
   23 FORMAT (///)
   24 FORMAT (10E12.5)
   25 FORMAT (1H0,'INITIAL CONDITIONS (YFS)',/)
   26 FORMAT (1H0,'XJH'/)
   31 FORMAT (1H0,' CC  MASS FRACTION (YC)'/)
   32 FORMAT (1H0,'SURFACE  CO  MASS FRACTION (YCS)'/)
   33 FORMAT (1H0,'INITIAL CONDITIONS (YCS)',/)
   34 FORMAT (1H0,' ES,S =    ', 6F12.6/)
   35 FORMAT (1H0,'  C,S =    ', 5E20.10/)
   36 FORMAT (1H0,'  A,S =    ', 6F12.6/)
   37 FORMAT (1H0,' BE,S =    ', 6F12.6/)
   41 FORMAT (1H0,' YCC =',/)
   42 FORMAT (1H0,' YCC(SURFACE) =',/)
   43 FORMAT (1H0,' L/U =', F15.7/)
   44 FORMAT (1H0,' B1S, B2S,  =', 4E15.8/)
   45 FORMAT(1H0,'B0-4 =',5E15.8/)
   46 FORMAT (4E20.8)
   47 FORMAT (1H0,' E,S =',6F12.6/)
   48 FORMAT (1H0,'GC, XLEN1, XLEN2, XLS, DS =',6F12.6 /)
   49 FORMAT(1H0,'RO1,  XK1, CP, ALPHA =', 3F12.6,E12.5/)
   71 FORMAT (1H0,'APPROACH VEL = ',F10.4/)
   72 FORMAT (1H0,'CHANNEL VEL (I.U.) = ',F10.5/)
   73 FORMAT(1H0,'EFFICIENCY(CARBON-BALANCE)',/)
  401 FORMAT (1H0,' XPI =', F20.5/)
  402 FORMAT (1H0,'TI, PR, REY, AD2UL, AGAS =',5F12.5/)
  403 FORMAT (1H0,' ES,S=',5E20.8/)
  404 FORMAT (1H0,'*********************************************',/)
  405 FORMAT (1H0,'GAS TEMPERATURE IS NEGATIVE')
  406 FORMAT (1H0,' CNHM CONCENTRATION IS NEGATIVE')
  407 FORMAT (1H0,'  CC  CONCENTRATION IS NEGATIVE')
  408 FORMAT (1H0,' YFF IS NEGATIVE')
  409 FORMAT(1H0,'ADIABATIC FLAME TEMP =',F10.6/)
  410 FORMAT(1H0,'ADIAB FLAME TEMP(K) =',F15.5/)
  411 FORMAT(1H0,'BETA 1-5 =',5F10.4/)
  412 FORMAT(1H0,'PYROLYZED CNHM (YE)',/)
  413 FORMAT(1H0,'TOTAL CNHM (YTHC)',/)
      ********************************************
```

```
7000          *****     INPUT PARAMETERS     *****
7100
7200          *****     CHEMICAL PARAMETERS     *****
7300
7400
7450          CHEMICAL REACTION 0,  CNHM = CNHM (GAS PHASE PYROLYSIS)
7475                                      (ISOTHERMAL REACTION)
7500          CHEMICAL REACTION 1,   CNHM + O2 = CO +H2O (GAS PHASE)
7600          CHEMICAL REACTION 2, CO + O2 = CO2 (GAS PHASE)
7700          CHEMICAL REACTION 3,  CNHM +O2 = CO2 + H2O ( SOLID SURFACE)
7800          CHEMICAL REACTION 4,  CO + O2 = CO2 (SOLID SURFACE)
7900
8000
8100          ES1 = ACTIVATION ENERGY FOR REACTION 1 (CAL/MOLE), ETC.
8200          C1 = PREEXPONENTIAL FACTOR (DIMENSIONAL) FOR REACTION 1, ETC.
8300          WHC, WCO = MOLECULAR WEIGHTS FOR CNHM, CO
8400          Q1S = HEAT OF COMBUSTION FOR REACTION 1 (CAL/G OF CNHM)
8500          Q2S = HEAT OF COMBUSTION FOR REACTION 2 (CAL/G OF CO)
8600          QS = HEAT OF COMBUSTION FOR REACTION 3 ( CAL/G OF CNHM)
8700          XN = THE NUMBER OF CARBONS IN CNHM
8800          XM = THE NUMBER OF HYDROGEN IN CNHM
8900
9000
9100
9200          QS = Q1S + Q2S*XN*WCO/WHC
9300
9400          *****     CATALYTIC BED PARAMETERS     *****
9500
9600          XLS = BED LENGTH  (M)
9700          DS = CHANNEL HYDRAULIC DIAMETER(M)
9800          SOA = CIRCUMFERENTIAL LENTH DIVIDED BY CHANNEL AREA,=4/DS (1/M)
9900           AOAS = RATIO OF OPEN TO CLOSED AREAS
10000         CSS = HEAT CAPACITY OF SUBSTRATE (CAL/KG/K)
10100         ROS= DESITY OF SUBSTRATE  (KG/ M3)
10200
10300
10400         READ(5,10)  XPHI
10500         READ (5,10)  TI
10600         READ (5,10)  XPI
10700         READ (5,10)  UIUS
10800         READ (5,10)  XLS
10900         READ (5,10)  DS
11000         READ (5,10)  AOAS
11100         READ(5,*) DXX, XAS
11200         READ (5,10)  DT
11300         READ (5,10)  TMAX
11400         READ(5,8)  N
11425          READ(5,8) NAS
11437         READ(5,8) IT
11450          READ(5,*) C0,C1,C2,C3,C4
11475         READ(5,8) IPUTIN
11500         SOA = 4.0/DS
11600         CN = XN*WCO/WHC
11650         NPNAS=N+NAS
11700
11800         *****     OPERATING PARAMETERS     *****
11900         TI = INITIAL, UPSTREAM (I.U.) TEMPERATURE (K)
12000         UI = I.U. VELOCITY (M/S)
12100         XPI = I. U. PRESSURE (ATM.)
12200         ROI= I.U. GAS DENSITY  (KG/M3)
12300         YFI = I.U. MASS FRACTION OF HC
12400         YCI = I.U. MASS FRACTION OF CC
12500         YOI = I.U. MASS FRACTION OF O2
12600         XPHI = UPSTREAM  HC/O2 EQUIVALENCE RATIO
12700
12800
12900          UI = UIUS*(1.0+AOAS)/AOAS
13000         XMU = 0.000001458*SQRT(TI)/(1.0+110.4/TI)
13100          YFI=WHC*XPHI/29./((XN+XM/4.)*4.76+XPHI)
13200         XLEW1 = 1.5* SQRT (29./WHC)
13300         XLEW2=1.5* SQRT(29./WCO)
13350         XLE123=XLEW1**.667
13375         XLE223=XLEW2**.667
13400
13500         XLOU = XLS/UI
13600
13700         *****     GAS PROPERTY     *****
13800
13900
14000         CP = SPECIFIC HEAT OF GAS (CAL/KG/K)
14100         XKI = HEAT CONDUCTIVITY OF GAS AT I.U. (CAL/ M/SEC/K)
```

```
14200         ALPHA = 1.U. GAS THERMAL DIFFUSIVITY ( M2/SEC)
14300         GC=GAS CONSTANT FOR GAS MIXTURE  (JOULE/KG/K)
14400         XLEW1 = LEWIS NUMBER FOR CNHM IN MIXTURE
14500         XLEW2 = LEWIS NUMBER FOR  CO  IN MIXTURE
14600
14700
14750         XKI=.003+.000013*TI
14800         ROI = XPI/GC/TI
14900         ALPHA = XKI/ROI/CP
15000         REY = UIUS*DS*RCI/XMU
15100
15200
15300         TO DESCRIBE CHEMICAL REACTION RATE EXPRESSIONS
15350         REACTION 0 (GAS PHASE ISOTHERMAL PYROLYSIS)
15375         D(CNHM)/DT $$$ (CNHM)/EXP(E0/RT)
15387
15400         REACTION 1 ( GAS PHASE )
15500         D(CNHM)/DT $$$ XP**.3*T*SQRT(YHC)*YO2/EXP(E1/RT)
15600
15700         REACTION 2 (GAS PHASE )
15800         D(CO)/DT $ P**BTA1*CO**BTA2*O2**BTA3*T**BTA4*H2O**BTA5/EXP(E2/RT)
15900
16000         REACTION 3 (SOLID SURFACE)
16100         D(CNHM)/DT $$$ YHCS/EXP(E3/RT)
16200
16300         REACTION 4 (SOLID SURFACE)
16400         D(CC)/DT $$$ YCCS/EXP(E4/RT)
16500
16600         TO EVALUATE  KINETIC RATE CONSTANTS.
16700
16750         B0=C0*XLOU*(WHC/ROI/YFI)**(1.-GAMA)
16800         B1SS = C1*SQRT(WHC)/WC2/SQRT(1000.)
16900         B1S = B1SS*XPI**.3*ROI*SQRT(ROI)*TI*SQRT(YFI)*YOI
17000         B1 = XLOU*B1S/RCI/YFI
17100         B235=BTA2+BTA3+BTA5
17150         C2M=C2*1000.**(1.-B235)
17200         B2SS=C2M*WCO**(1.-BTA2)/(WO2**BTA3*WH2O**BTA5)
17300         B2S=B2SS*XPI**BTA1*ROI**B235*TI**BTA4*YFI**BTA2*YOI**BTA3
17400         B2 = B2S*XLOU/RCI/YFI
17500
17900         B3=C3*DS/ALPHA/WHC/3.66
17950         B4=C4*DS/ALPHA/WCO/3.66
18000         Q1 = Q1S/CP/TI
18100         Q2 = Q2S/CP/TI
18200         Q = QS/CP/TI
18250         TAB=YF1*Q+1.0
18275         TABDM=TAB*TI
18287         E0= ES0/TI/1.987
18300         E1= ES1/TI/1.987
18400         E2= ES2/TI/1.987
18500         E3= ES3/TI/1.987
18600         E4= ES4/TI/1.987
18700         AD2UL = (ALPHA/DS/DS) /(UI/XLS)
18800         **********************************
18900
19000         WRITE (6,21) N,NAS
19100         WRITE(6,20) TMAX
19200         WRITE (6,15) YCI, YF1, XPHI
19300         WRITE(6,71) UIUS
19400         WRITE (6,72) UI
19500         WRITE (6,17) Q1, Q2, DXX, DT
19600         WRITE (6,402)TI,XPR,REY, AD2UL, AOAS
19650         WRITE(6,409) TAB
19675         WRITE(6,410) TABDM
19700         WRITE (6,403)ES0,ES1,ES2,ES3,ES4
19800         WRITE(6,47)E0,E1,E2,E3,E4
19900         WRITE(6,35)C0,C1,C2,C3,C4
19950         WRITE (6,411) BTA1,BTA2,BTA3,BTA4,BTA5
20000         WRITE (6, 40) GC, XLEW1, XLEW2, XLS, DS
20100         WRITE (6,49) ROI,        XKI, CP, ALPHA
20200         WRITE (6,401) XPI
20300         WRITE (6,43) XLOU
20400         WRITE (6,44) B1S, B2S
20500         WRITE(6,45)B0,B1,B2,B3,B4
21100
21200
21300         ******************************************
21400
21500         ********     UPSTREAM CONDITIONS
21600         YF(1)=1.
21650         YE(1)=0.
```

```
21700          YC(1)  = 0.0
21800          YO(1)=1.
21900          T(1)=1.
22000          RO(1)=1.
22100          XP(1) =1.0
22200          U(1)=1.
22250          YTHC(1) = YF(1)+YE(1)
22300
22400          ****************************************
23000
23100          ****************************************
23200          START OF INTEGRATION LOOP
23300          KOUNT = 1
23350          XNU0=.885*SQRT(ACAS)*SQRT(XPR*REY)
23375          ROOT1=0.0
23387          ROOT2=1.0
23393      555 ROOT=.5*(ROOT1+ROOT2)
23396          IF(ROOT.LE.0.1) YNU=.0444/ROOT+3.46-1.34*ROOT
23397          IF(ROOT.GT.0.1) YNU=0.011/ROOT+3.66
23398          YROOT=YNU-XNU0
23449          IF(ABS(YROOT).LT.0.01) GO TO 200
23474          IF(YROOT.GT.0.0) ROOT1=ROOT
23487          IF(YROOT.LE.0.0) ROOT2=ROOT
23493          GO TO 555
23500      200 CONTINUE
23550          DMASS=RO(1)*U(1)
23600
23700          INTEGRATION OF QUASI-STEADY GAS PHASE EQUATIONS FOR
23800          YF (FUEL MASS FRACTION) AND T ( TEMPERATURE ) IN DOWNSTREAM
23900          DIRECTION USING FOURTH-ORDER RUNGE-KUTTA SCHEME
24000          I IS THE INDEX FOR DOWNSTREAM DISTANCE X
24100
24200
24300          DO 201 I=1,NPNAS
24350
24362          IF(I.LE.N) DX=DXX
24374          IF(I.GT.N) DX=XAS*DXX
24375          IF(I.GT.N)DMASS=RO(1)*U(1)*ACAS/(ACAS+1.)
24400          ********************************
24500
24600          EVALUATE XJH AND XJD AS A FUNCTION OF X
24700
24800          **********************
24900          NONDIMENSIONAL HEAT CONDUCTIVITY
25000          XK = (.003+ 0.0000013* TI *I(I)) /XK1
25100          **********************
25200
25300          IF(I.GT.1) GO TO 180
25325          IF(I.EQ.1) X=0.0
25337          GO TO 181
25349      180 CONTINUE
25350          IX=I+1
25450          XI=IX-1
25500          X  = XI*DX
25550      181 CONTINUE
25600          XST= X*2.0*AD2UL*XK+ROOT
25700          IF(XST.LE.0.1) XNU=0.0444/XST+3.46 -1.34*XST
25800          IF(XST.GT.0.1) XNU=0.011/XST +3.66
26250          RNK(I)=XNU*XK/3.66
26300          XJH(I)   = 4.0*XNU *AD2UL*XK
26350          IF(I.GT.N) XJH(I) =0.0
26400          XJD1(I) = XJH(I) *XLE123
26500          XJD2(I) = XJH(I) *XLE223
26600          ********************************
26700
26800      132 CONTINUE
26900          M=1
27000          DO 120 L=1,4
27100          IF (M.NE.1) GO TO 102
27200          YFF= YF(I)
27250          YEE =YE(I)
27300          YCC =YC(I)
27400          TT = T(I)
27500          M=M+1
27600          GO TO 119
27700      102 CONTINUE
27800          IF (M.NE.2)  GO TO 103
27900          YFF=YF(I)+DX*XKY(1) /2.
27950          YEE=YE(I)+DX*XKE(1)/2.
28000          YCC =YC(I) +DX*XKC(1)/2.
28100          TT  =T(I)+DX*XKT(1) /2.
```

```
28200          M=M+1
28300          GO TO 119
28400      103 CONTINUE
28500          IF(M.NE.3) GO TO 104
28600          YFF = YF(1) +DX*XKY(2) /2.
28650          YEE= YE(I)+DX*XKE(2)/2
28700          YCC =YC(I) +DX*XKC(2)/2.
28800          TT=T(I)+DX*XKT(2) /2.
28900          M=M+1
29000          GO TO 119
29100      104 CONTINUE
29200          YFF = YF(I) + DX*XKY(3)
29250          YEE= YE(I) +DX*XKE(3)
29300          YCC =YC(I) +DX*XKC(3)
29400          TT=T(I) +DX*XKT(3)
29500      119 CONTINUE
29600          YH2O = MASS FRACTION OF H2O
29700          YH2O(I) = .5*XM*WH2O*YFI* (YTHC(1)-YTHC(I))/WHC
29800          IF (YFF.LT.0.0) YFF=0.0
29850          W0=B0*(RO(I)*YFF)**GAMA/EXP(E0/TT)
29875          IF(YEE.LT.0.0) YEE=0.0
29900          W1 = B1* XP(I)**.3*RO(I)*SQRT(RO(I))*T(I)*SQRT(YEE) *YO(I)
30000         1  /EXP(E1/TT)
30025          IF(YCC.LT.0.0) YCC=0.0
30050          SSYO=YO(I)**BTA3
30075          RO235=RO(1)**B235
30100          W2=B2*RO235*SSYC*YCC**BTA2*YH2O(I)**BTA5*XP(I)**BTA1/EXP(E2/TT)
30200          XKY(L) = -XJD1(I) *(YFF- YFS(I))/DMASS -W0/DMASS
30250          XKE(L)=-XJD1(I)*(YEE-YES(I))/DMASS+(W0-W1)/DMASS
30300          XKC(L) = -XJD2(I) *(YCC-YCS(I))/ DMASS +CN*W1/DMASS -W2/DMASS
30400          XKT(L) =-XJH(I)*(TT-TS(I))/DMASS +Q1*YFI*W1/DMASS+Q2*YFI*W2/DMASS
30500      120 CONTINUE
30600          YF(I+1) =YF(I) +DX*(XKY (1)/6. +XKY (2)/3. +XKY (3)/3.+XKY (4)/6.)
30700          IF (YF(I+1).LT.0.0) YF(I+1) =0.0
30750          YE(I+1)=YE(I)+DX*(XKE(1)/6.+XKE(2)/3.+XKE(3)/3.+XKE(4)/6.)
30775          IF(YE(I+1).LT.0.0) YE(I+1)=0.0
30800          YC(I+1) =YC(I) +DX*(XKC (1)/6. +XKC (2)/3. +XKC (3)/3.+XKC (4)/6.)
30900          IF (YC(I+1).LT.0.0) YC(I+1) =0.0
31000          T (I+1) =T (I) +DX*(XKT (1)/6. +XKT (2)/3. +XKT (3)/3.+XKT (4)/6.)
31100          IF (T(I+1).LT..0) GO TO 601
31125          YTHC(I+1)=YF(I+1)+YE(I+1)
31150          ADD=YC(I+1)*YFI*WO2/YCI/WCC/2.
31200          YO(I+1) =1.0-XPHI*(1.0-YF(I+1))+ADD
31300          XP(I+1)=XP(I)
31400          RO(I+1)=XP(I+1) /T(I+1)
31500          U(I+1) =DMASS/T(I+1)
31550           EFF(I)=1.-YTHC(I)-YC(I)*Q2/Q
31600      201 CONTINUE
31700
31800          END OF ONE RUNGE-KUTTA INTEGRATION CYCLE FOR QUASI-STEADY
31900          GAS PHASE EQUATIONS
32000          ******************************************
32100
32200
32300          ******************************************
32400          INTEGRATION OF UNSTEADY SOLID HEAT TRANSFER EQUATION
32500          FOR TS ( SOLID TEMPERATURE ) IN TIME USING  FOURTH-ORDER
32600          RUNGE-KUTTA SCHEME
32700
32800
32900
33000          DO 301 J =1,N
33100          MJ=1
33200          DO 320  LJ=1,4
33300          IF (MJ.NE.1) GO TO 302
33400          TSS =TS(J)
33500          MJ=MJ+1
33600          GO TO 319
33700      302 CONTINUE
33800          IF(MJ.NE.2)  GO TO 303
33900          TSS = TS(J) + DT*XKTS(1)/2.
34000          MJ=MJ+1
34100          GO TO 319
34200      303 CONTINUE
34300          IF(MJ.NE.3)  GO TO 304
34400          TSS=TS(J)+DT*XKTS(2) /2.
34500          MJ=MJ+1
34600          GO TO 319
34700      304 CONTINUE
34800          TSS = TS(J) + DT* XKTS(3)
34900      319 CONTINUE
```

```
34950          YFSES=YFS(J)+YES(J)
35000          XKTS(LJ)=RNK(J)*(T(J)-TSS) +B3*YFI*Q*RO(J)*YFSES/EXP(E3/TSS)
35100         1 +B4*YFI*Q2*RO(J)*YCS(J)/EXP(E4/TSS)
35200      320 CONTINUE
35300          TS(J) =TS(J) +DT*(XKTS(1)/6.+XKTS(2)/3.+XKTS(3)/3.+XKTS(4)/6.)
35400          YFS(J) = YF(J) /(1.+B3*RO(J)/XLE123/RNK(J)/EXP(E3/TS(J)))
35450          YES(J)=YE(J)/(1.+B3*RO(J)/XLE123/RNK(J)/EXP(E3/TS(J)))
35500          YCS(J) = YC(J) /(1.+B4*RO(J)/XLE223/RNK(J)/EXP(E4/TS(J)))
35600      301 CONTINUE
35700
35800          END OF ONE TIME INTEGRATION STEP
35900          ********************************************
36000
36100          ********************************************
36200          LOOP FOR MARCHING FORWARD IN TIME
36300
36400          KOUNT =KOUNT+1
36500          KOU   =KOUNT-1
36600          XKOUNT =KOUNT
36700          TIME=(XKOUNT-1.)*DT
36800          IF (TIME.GT. TMAX) GO TO 999
36900          TIMER=TMAX-DT
36950          IF(TIME.LT.TIMER) GO TO 200
37000          WRITE(6,22) TIME  ,KOUNT
37100          WRITE (6,13)
37200          WRITE(6,24) (T  (I),I=1,NPNAS,IT)
37300          WRITE (6,9)
37400          WRITE(6,24) (TS (I),I=1,N,IT)
37500          WRITE(6,14)
37600          WRITE(6,24)  (YF(I),I=1,NPNAS,IT)
37650          WRITE(6,412)
37675          WRITE(6,24) (YE(I),I=1,NPNAS,IT)
37687          WRITE(6,413)
37699          WRITE(6,24) (YTHC(I),I=1,NPNAS,IT)
37700          WRITE(6,41)
37800          WRITE(6,24)  (YC(I),I=1,NPNAS,IT)
37900          WRITE(6,11)
38000          WRITE(6,24)  (YFS(I),I=1,N,IT)
38100          WRITE(6,42)
38200          WRITE(6,24)  (YCS(I),I=1,N,IT)
38300          WRITE(6,26)
38400          WRITE(6,24) (XJH(I),I=1,N,IT)
38500          WRITE(6,73)
38543          WRITE(6,24)  (EFF(I),I=1,NPNAS,IT)
38586          WRITE(6,23)
38593      901 CONTINUE
38594          IF(IPUTIN.EQ.1) GO TO 200
38596          OPEN(UNIT=11,TYPE='NEW',NAME='SOLID')
38599          WRITE (11,*) A
38624          CLOSE (UNIT=11)
38650          GO TO 200
38700
38800          END OF WHOLE INTEGRATION LOOP
38900          ********************************************
39000
39100      601 CONTINUE
39200          WRITE (6,404)
39300          WRITE(6,405)
39400      999 CONTINUE
39500          STOP
39600          END
```

```
  100         BLOCK DATA
  200
  300         DIMENSION TS(300),YFS(300),YCS(300),YES(300)
  400         COMMON /ACTI/ES0,ES1,ES2,ES3,ES4
  600         COMMON /MOLEQ/ WHC, WCO, WO2, WH2O
  700         COMMON /TH1/XN, XM, Q1S, Q2S
  800         COMMON /TH2/ CP, GC,  XPR
  900         COMMON /UPST/ YCI , YOI
 1100         COMMON /INI/TS,YFS,YCS,YES
 1150         COMMON /B12345/BTA1,BTA2,BTA3,BTA4,BTA5
 1175         COMMON /GAMMA/GAMA
 1200
 1400         DATA ES0,ES1,ES2,ES3,ES4/34000.,24000.,40000.,10000.,17800./
 1500         DATA WHC,WCO,WO2,WH2O/130.,28.,32.,18./
 1600         DATA XN,XM,Q1S,Q2S/10.,18.,5357000.,2415000./
 1700         DATA CP,GC,XPR/285.,2.8312E-3,0.7/
 1800         DATA YCI,YOI/0.,0.23/
 1900         DATA BTA1,BTA2,BTA3,BTA4,BTA5/0.,1.,0.25,0.,0.5/
 1950         DATA GAMA/0.5/
 2000         DATA TS,YFS,YCS,YES/300*1.,300*0.,300*0.,300*0./
 2100         END
```

Example calculation:

```
$ RUN CALY1.EXE;61
.165
1000.
3.
15.
.1
.001382
13.29
.01 1.
.1
8.001
  51
 100
   5
1.6E6 1.8E5 .54E14 1.5E4 1.E5
   1
```

Read-in data: ϕ, TI, XPI, UIUS, XLS, DS, AOAS, DXX, XAS, DT, TMAX, N, NAS, IT, C0, C1, C2, C3, C4, IPUTIN

```
NO. OF GRID POINT =        51       100


TMAX =       8.00100040

YO(UPST,INI) =  0.230000     YF (UPST,INI) = 0.0113489     EQUI RATIO =     0.165
000007


APPROACH VEL =     15.0000

CHANNEL VEL (I.U.) =    16.12867

Q1=      18.7964916      Q2=       8.4736843      DX=       0.0100000      DT=       0.
1000000


TI, PR, REY, AD2UL, ADAS =  1000.00000     0.70000   529.01978     0.17199    13
.29000

ADIABATIC FLAME TEMP =  1.408440

ADIAB FLAME TEMP(K) =      1408.44019
```

```
 ES,S=       0.34000000E+05       0.24000000E+05       0.40000000E+05       0.100000
00E+05       0.17800000E+05

 E,S =    17.111223    12.078510    20.130850     5.032712     8.958228

  C,S =         0.1600000000E+07     0.1800000000E+06     0.5399999886E+14     0.1500
000000E+05     0.1000000000E+06

BETA 1-5 =     0.0000     1.0000     0.2500     0.0000     0.5000

GC, XLEW1, XLEW2, XLS, DS =     0.002831     0.687624     1.526551     0.100000     0
.001382

PDI,  XKI, CP, ALPHA =     1.059621     0.016000  285.000000 0.52982E-04

 XPI =              3.00000

 L/U =       0.0062001

 B1S, B2S,  = 0.77647750E+05 0.26173910E+09

B0-4 = 0.10626966E+07 0.40033785E+05 0.13494798E+09 0.77466638E+03 0.25453324E+0
5

TIME=      8.00000000      KOUNT=          81

GAS TEMPERATURE (T)

0.10000E+01 0.10933E+01 0.11328E+01 0.11648E+01 0.11927E+01 0.12180E+01 0.12416E
+01 0.12640E+01 0.12855E+01 0.13063E+01
0.13262E+01 0.13387E+01 0.13506E+01 0.13629E+01 0.13739E+01 0.13806E+01 0.13853E
+01 0.13891E+01 0.13923E+01 0.13948E+01
0.13969E+01 0.13985E+01 0.13998E+01 0.14008E+01 0.14016E+01 0.14022E+01 0.14027E
+01 0.14031E+01 0.14034E+01 0.14036E+01
0.14038E+01

SOLID TEMPERATURE (TS)

0.11286E+01 0.13193E+01 0.13325E+01 0.13421E+01 0.13502E+01 0.13576E+01 0.13646E
+01 0.13713E+01 0.13779E+01 0.13842E+01
0.13901E+01

ORIGINAL CNHM (YF)

0.10000E+01 0.76186E+00 0.65814E+00 0.57097E+00 0.49212E+00 0.41866E+00 0.34867E
+00 0.28172E+00 0.21825E+00 0.15913E+00
0.10576E+00 0.65733E-01 0.33518E-01 0.10262E-01 0.16875E-03 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00
```

PYROLYZED CNHM (YE)

0.00000E+00 0.37022E-02 0.91331E-02 0.15642E-01 0.22801E-01 0.30127E-01 0.37036E
-01 0.42908E-01 0.47042E-01 0.48627E-01
0.46778E-01 0.44312E-01 0.36474E-01 0.22910E-01 0.59886E-02 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00

TOTAL CNHM (YTHC)

0.10000E+01 0.76556E+00 0.66727E+00 0.58662E+00 0.51493E+00 0.44878E+00 0.38571E
+00 0.32463E+00 0.26529E+00 0.20776E+00
0.15254E+00 0.11004E+00 0.69992E-01 0.33172E-01 0.61574E-02 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E
+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00

YCO =

0.00000E+00 0.16567E-02 0.65324E-02 0.15098E-01 0.27740E-01 0.44585E-01 0.65277E
-01 0.89093E-01 0.11487E+00 0.14085E+00
0.16454E+00 0.21374E+00 0.26066E+00 0.28957E+00 0.28939E+00 0.24645E+00 0.19836E
+00 0.15831E+00 0.12542E+00 0.98769E-01
0.77393E-01 0.60398E-01 0.46983E-01 0.36453E-01 0.28226E-01 0.21821E-01 0.16848E
-01 0.12996E-01 0.10017E-01 0.77166E-02
0.59417E-02

SURFACE HC MASS FRACTION (YFS)

0.59588E+00 0.55527E-01 0.41276E-01 0.33799E-01 0.28303E-01 0.23840E-01 0.20075E
-01 0.16396E-01 0.12835E-01 0.94545E-02
0.63485E-02

YCO(SURFACE) =

0.00000E+00 0.12246E-03 0.40424E-03 0.86451E-03 0.15176E-02 0.23790E-02 0.34733E
-02 0.47282E-02 0.60816E-02 0.74420E-02
0.86843E-02

XJH

0.42719E+02 0.39692E+01 0.33866E+01 0.31814E+01 0.30823E+01 0.30479E+01 0.30827E
+01 0.31189E+01 0.31556E+01 0.31922E+01
0.32283E+01

EFFICIENCY(CARBON-BALANCE)

0.00000E+00 0.23405E+00 0.33119E+00 0.40983E+00 0.47854E+00 0.54072E+00 0.59893E
+00 0.65439E+00 0.70766E+00 0.75908E+00
0.80872E+00 0.83963E+00 0.86864E+00 0.89865E+00 0.92571E+00 0.94197E+00 0.95330E
+00 0.96273E+00 0.97047E+00 0.97674E+00
0.98178E+00 0.98578E+00 0.98894E+00 0.99142E+00 0.99335E+00 0.99486E+00 0.99603E
+00 0.99694E+00 0.99764E+00 0.99818E+00
0.99860E+00

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16. Abstract

A quasisteady-gas-phase and thermally-thin-substrate model is used to analyze the transient behavior of catalytic monolith combustors in fuel-lean operation. The combustor response delay is due to the substrate thermal inertia. Fast response is found to be favored by thin substrate, short catalytic bed length, high combustor inlet and final temperatures and, in most cases, small gas channel diameters. The calculated gas and substrate temperature time history at different axial positions provides an understanding of how the catalytic combustor responds to an upstream condition change. The computed results also suggest that the gas residence times in the catalytic bed and in the after-bed space are correlatable with the nondimensional combustor response time. The model can also perform steady-state combustion calculations; and the computed steady-state emission characteristics show good agreement with available experimental data in the range of parameters covered. From combined steady and unsteady considerations, it is possible to choose a catalytic combustor design for automotive gas turbine engine which has reasonably fast response (< 1 second) and can satisfy the emission goals in an acceptable total combustor length.

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