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Assessment of a Modular Ramjet Combustor Model

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Several advanced ramjet combustor concepts utilize sudden-expansion geometries in which the step acts as a flameholding device. Flame stabilization and flame propagation problems have been encountered in these types of combustors. To aid in assessing these problems, analytical models of the recirculation region downstream of the step have been developed and incorporated in a ramjet performance prediction model. The use of this model to analyze and interpret the performance characteristics of a sudden-expansion combustor is described in this paper, with particular emphasis on the modeling of the flame stabilization region. It is shown that the approach provides an accurate and efficient means of verifying suspected causes of ramjet combustor performance deficiencies.

Nomenclature

a,b = coefficients in shear layer width relationship, Eq. (7)
C_{E_1}, C_{E_2} = turbulent kinetic energy dissipation rate coefficients, Eq. (15)
C_μ = turbulent eddy viscosity coefficient
h = static enthalpy
H = total enthalpy
k = turbulent kinetic energy
l = shear layer width or fuel penetration distance
$\dot{m}$ = mass flow rate
M = total mass contained in well-stirred reactor volume
p = pressure
Pr = turbulent Prandtl number
$\dot{Q}$ = rate of heat addition to well-stirred reactor
r = radial coordinate
r_0 = combustor inlet radius
R = universal gas constant
R_c = radial coordinate of recirculation region dividing streamline
s = path variable along dividing streamline
Sc = turbulent Schmidt number
t = time
T = temperature
u = axial velocity component
v = radial velocity component
V = stirred reactor volume
$\dot{w}$ = volumetric production rate due to chemical reaction
W = molecular weight
x = axial coordinate
α = species mass fraction
ϵ = turbulent kinetic energy dissipation rate
κ = thermal conductivity
μ_T = turbulent dynamic viscosity
ρ = density
σ_K = turbulent exchange coefficient for turbulent kinetic energy
σ_ϵ = turbulent exchange coefficient for turbulent kinetic energy dissipation rate
ν_T = turbulent kinematic viscosity $= \mu_T/\rho$
ϕ = generalized dependent variable

Subscripts and Superscripts

c = characteristic value in recirculation region
i = individual specie
I = inflow to recirculation region
O = outflow from recirculation region
P = condition immediately outside recirculation zone
R,RZ = conditions within recirculation zone
W = condition along dividing streamline

Introduction

INCREASED demand for higher performance from air-breathing propulsion systems in general, and ramjet devices in particular, has resulted in the need to upgrade existing technologies to meet more stringent design requirements. Reducing combustor volume and weight involves the use of shorter combustors and high energy, high density fuels. Furthermore, system constraints have dictated the use of sudden-expansion (dump) combustors capable of operating effectively at high combustion intensities over wide ranges of conditions. However, flame stabilization, flame propagation, and spray combustion problems have been encountered in the development of dump combustors. To aid in obtaining solutions to these problems, analytical combustor models are a requirement: the ability to compute in some detail combustion chamber flowfields is necessary in order to understand the phenomena that occur in existing combustors and to predict the performance of new combustor concepts. The insight gained through the use of analytical combustor models can be of substantial value in the planning of a combustor test program and in the interpretation of combustor and combustor component test data.

In response to the needs just outlined, a detailed model of the sudden-expansion liquid fueled ramjet combustor has been developed, as reported in Refs. 1-3. This model makes use of the modular concept, in which the combustor flowfield, represented schematically in Fig. 1, is broken down into three major components: a directed flow, which is treated as parabolic, a recirculation zone, assumed to be represented by well-stirred reactor(s), and a turbulent shear layer along the dividing streamline which separates the other two regions. The shear layer serves as the coupling region between the other two model components; fluxes of species and energy

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across this shear layer form the boundary conditions on the two computational regions. Finite-rate chemistry, based on the quasiglobal model[4] is included in the formulations for both the directed-flow and well-stirred reactor regions, although for the modular model calculations described in this paper, the recirculation region well-stirred reactor formulation has been restricted to a global finite-rate chemistry model. The directed flow is assumed to be fully turbulent, with the turbulent viscosity defined by a two-equation turbulence model.[5] A key feature of this approach is the provision for the shear layer coupling region. Through the use of this element of the model, the division of the mass flux between the directed-flow and the recirculation region is computed iteratively rather than specified empirically. Furthermore, the directed-flow region is computed as a two-dimensional parabolic flowfield, rather than using a one-dimensional approximation, allowing detailed computation of the mixing and chemical reactions in this region of the combustor.

A variety of results obtained in the process of validating the modular model approach have been described in Ref. 1; in general these results bear on the validation of the performance prediction aspect of the model. In this paper, the use of the model in the interpretation of ramjet combustor test data is discussed, with particular emphasis on the interaction of the flame stabilizing recirculation zone with other aspects of the combustor flowfield.

Stirred Reactor Modeling of Dump Combustor Recirculation Zones

The well-stirred reactor, shown schematically in Fig. 2a, is a laboratory device in which very high mixing rates are achieved. In general, laboratory stirred reactors are designed to ensure that the mixture within the reactor is spatially uniform, so that unreacted feed material is continuously and uniformly mixed with combustion products, reacting for a time defined by the average residence time of the reactor before exiting. For the limit of perfect stirring, this average residence time is given simply by the ratio of the product of the stirred reactor volume and density to the feed mass flux, $\rho V/\dot{m}$; the product mass flux is of course equal to the feed mass flux. In this limit the governing equations for the stirred reactor state reduce to algebraic relations,[6] which allows the use of rapid and efficient solution procedures, incorporating either global finite-rate kinetics or the more detailed quasiglobal kinetics formulation.

In the lower half of Fig. 2, a typical recirculation region in a sudden-expansion combustor is sketched. Because of the high turbulence intensity and large mixing rates generated in the recirculation zone, the limiting behavior of this region can be thought of as well-mixed; that is, the state of the recirculation region is defined by the chemical kinetics of the reactions occurring and not by the mixing rate. In this sense the volume within the recirculation region sketched in Fig. 2b is similar to the volume within the laboratory stirred reactor of Fig. 2a, and the same solution technique can be used to obtain the thermochemical state. A comparison of Figs. 2a and 2b also shows the major difference between the recirculation region and the laboratory stirred reactor. In the laboratory stirred reactor, discrete reactant and product streams can be identified, but in the well-stirred reactor model of a sudden-expansion recirculation zone, separate reactant and product streams cannot be defined. Instead, reactants enter and products leave the recirculation region by turbulent diffusion through the shear layer which surrounds the dividing streamline. Thus the reactant stream is the flux of reactants passing through the shear layer, integrated over the surface area of the dividing stramline, and the product stream is defined similarly. These fluxes are of course equal and opposite.

The equations describing the transport of energy and species in the well-stirred reactor reduce to the following relations:

Continuity,

$$\dot{m}^I = \dot{m}^O = \dot{m} \tag{1}$$

Species,

$$\frac{\mathrm{d}M\alpha_i}{\mathrm{d}t} = \dot{m}_i^I + V\dot{w}_i \tag{2}$$

Energy,

$$h = \sum_i h_i\alpha_i = h^I + \dot{Q}/\dot{m} \tag{3}$$

Note that in this set of equations the species transport equation is written in nonsteady form. This formulation has been adopted to facilitate solution of the stirred reactor governing equations with finite-rate chemical kinetics; the steady-state stirred reactor solution is obtained when $\mathrm{d}\alpha_i/\mathrm{d}t \to 0$.

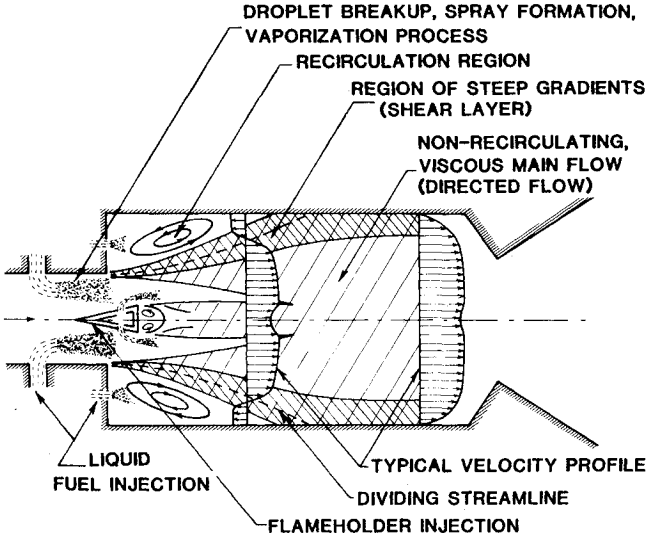

Fig. 1 Schematic of sudden-expansion (dump) burner.

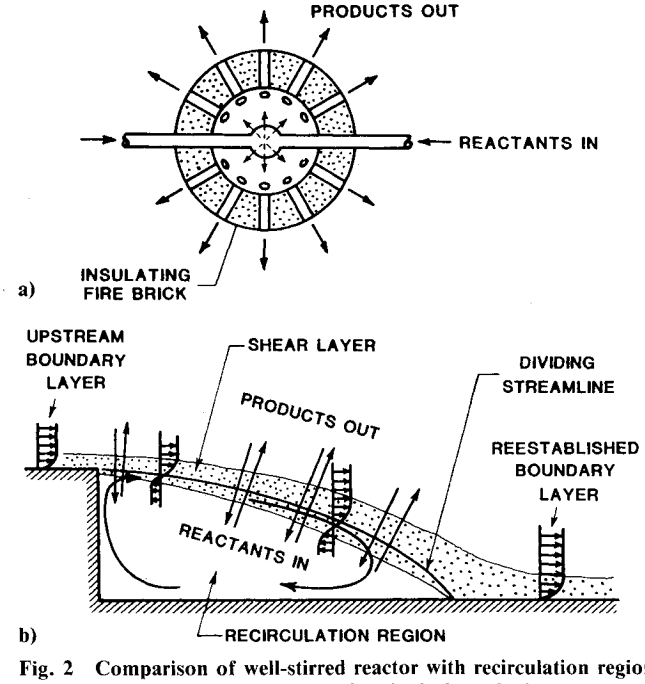

Fig. 2 Comparison of well-stirred reactor with recirculation region flowfield: a) schematic design of spherical well-stirred reactor; b) schematic of sudden-expansion recirculation region.

Equations (1-3), along with expressions for the volumetric species production rates, for the enthalpy of individual species as a function of temperature, and the equation of state, define the temperature and species concentrations in the stirred reactor, given the inflow rates for species and enthalpy. In the modular model, the net inflow of species and enthalpy are each expressed as line integrals involving gradients evaluated along the dividing streamline, so that the energy and species conservation equations for the stirred reactor are written, respectively,

$$-2\pi\int_0^s R_c(x)\rho\nu_T \sum\left[h_i^I(T^I)\frac{\partial\alpha_i^I}{\partial r}\right]ds+\dot{Q}$$
$$=2\pi\int_0^s R_c(x)\kappa\frac{\partial T}{\partial s}\,ds$$
$$-2\pi\int_0^s R_c(x)\rho\nu_T \sum_i\left[h_i^O(T_R)\frac{\partial\alpha_i^O}{\partial r}\right]ds \tag{4}$$

and

$$\frac{d\alpha_i}{dt}=\frac{-2\pi}{\rho_c V}\int_0^s R_c(x)\left[\rho\nu_T\frac{\partial\alpha_i^I}{\partial r}\right]ds$$
$$-\frac{2\pi}{\rho_c V}\int_0^s R_c(x)\left[\rho\nu_T\frac{\partial\alpha_i^O}{\partial r}\right]ds+\frac{\dot{w}_i}{\rho_c} \tag{5}$$

where $\rho\nu_T$ is evaluated using the outer flowfield solution in the region of the dividing streamline.

Because in the modular model the feed rates into the recirculation region are defined by the fluxes of reactants and products through the shear layer, this region becomes a key element of the model. Nevertheless, the shear layer is modeled simply as a region of linear gradients; that is, the gradient in a quantity ϕ at the dividing streamline is approximated by

$$\left(\frac{\partial\phi}{\partial r}\right)_w=\frac{\phi_P-\phi_R}{l} \tag{6}$$

Moreover, the width of the shear layer is assumed to be given by the linear expression

$$l=ax+b \tag{7}$$

in which a and b are defined through comparison of model predictions with experimental data. The results obtained with the modular approach have been found[1] to be relatively insensitive to the values of the coefficients a and b in Eq. (7); for the results presented in this paper, $a=0.03$ and $0.07<b<0.09$.

Parabolic Mixing: The Directed-Flow Model

The second major element of the modular model for a sudden-expansion combustor is the formulation for the directed-flow portion of the combustor flowfield. It is assumed that the boundary-layer approximations apply to this part of the flowfield. For a steady, axisymmetric flow, the describing equations may be written as follows:

Global Continuity,

$$\frac{\partial r\rho u}{\partial x}+\frac{\partial r\rho v}{\partial r}=0 \tag{8}$$

Species Diffusion for the ith Specie,

$$\rho u\frac{\partial\alpha_i}{\partial x}+\rho v\frac{\partial\alpha_i}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left\{r\rho\frac{\nu_T}{Sc}\left[\frac{\partial\alpha_i}{\partial r}\right]\right\}+\dot{w}_i \tag{9}$$

Momentum Equation,

$$\rho u\frac{\partial u}{\partial x}+\rho v\frac{\partial u}{\partial r}=\frac{1}{r}\left\{\frac{\partial}{\partial r}\left(r\rho\nu_T\frac{\partial u}{\partial r}\right)\right\}-\frac{\partial p}{\partial x} \tag{10}$$

Energy Equation,

$$\rho u\frac{\partial H}{\partial x}+\rho v\frac{\partial H}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left\{\frac{r\rho\nu_T}{Pr}\left[\frac{\partial H}{\partial r}-\left(\frac{Pr}{Sc}-1\right)\right.\right.$$
$$\left.\left.\sum_i h_i\frac{\partial\alpha_i}{\partial r}+(Pr-1)\frac{\partial}{\partial r}\left(\frac{u^2}{2}\right)\right]\right\} \tag{11}$$

These equations, along with expressions for the enthalpy

$$H=h+(u^2/2)\quad\text{and}\quad h=\sum_i\alpha_i h_i(T) \tag{12}$$

and the equation of state

$$p=\rho RT\sum_i(\alpha_i/W_i) \tag{13}$$

can be solved, given an expression for the turbulent eddy viscosity $\mu_T=\rho\nu_T$. This is defined by a two-equation turbulent kinetic energy model,[5] which introduces transport equations for the turbulent kinetic energy and its dissipation rate. In boundary-layer form, these equations can be written as follows:

Turbulent Kinetic Energy

$$\rho u\frac{\partial k}{\partial x}+\rho v\frac{\partial k}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\mu_T r}{\sigma_k}\frac{\partial k}{\partial r}\right)+\mu_T\left(\frac{\partial u}{\partial r}\right)^2-\rho\epsilon \tag{14}$$

Turbulence Energy Dissipation,

$$\rho u\frac{\partial\epsilon}{\partial x}+\rho v\frac{\partial\epsilon}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\mu_T r}{\sigma_\epsilon}\frac{\partial\epsilon}{\partial r}\right)+C_{E1}\frac{\epsilon}{k}\mu_T\left(\frac{\partial u}{\partial r}\right)^2-C_{E2}\rho\frac{\epsilon^2}{k} \tag{15}$$

where $\mu_T=C_\mu\rho k^2/\epsilon$. A standard set of two-equation model coefficients has been used for all of the computations reported in this paper: thus $C_\mu=0.09$, $C_{E1}=1.40$, $C_{E2}=1.95$, $\sigma_k=1.00$, and $\sigma_\epsilon=1.22$.

Chemical Kinetics: The Quasiglobal Model

In both the stirred reactor and directed-flow portions of the modular model, volumetric chemical kinetic production rate terms appear in the species transport equations. These terms can be evaluated using a full hydrocarbon chemical kinetics scheme based on the quasiglobal kinetics model,[4] which has as a key element a subglobal oxidation step

$$C_nH_m+(n/2)O_2\rightarrow(m/2)H_2+nCO \tag{16}$$

This reaction is unidirectional with an empirically determined rate (grams of fuel per cubic centimeter per second) given by

$$\frac{d[C]_{C_nH_m}}{dt}=AT^b p^{0.3}[C_nH_m]^{1/2}[O_2]\exp[-E/RT] \tag{17}$$

with the constants, A, b, and E/R defined in Table 1, where p must be given in atmospheres, T in degrees Kelvin, and [ ] denotes molar concentration; coupled to this subglobal step are the intermediate reversible reactions also given in Table 1.

Overall Computational Procedure

A flowfield computation using the modular model proceeds as follows: A dividing streamline shape is assumed, and the shear layer width expression and shear stress distribution along the dividing streamline are specified, the latter through use of a specified "skin friction" coefficient.[1-3,6] An initial state for the stirred reactor is assumed, which defines an initial guess for the species distribution and temperature within the recirculation zone. With these available as

Table 1 Extended C-H-O chemical kinetic reaction mechanism $k_f = AT^b \exp(-E/RT)$[a]

Reaction		A	b Forward	E/R
$C_nH_m + (n/2)O_2 \rightarrow (m/2)H_2 + nCO$	a) Long chain	6.0×10^4	1	12.2×10^3
	b) Cyclic	2.08×10^7	1	19.65×10^3
$CO + OH = H + CO_2$		5.6×10^{11}	0	0.543×10^3
$CO + O_2 = CO_2 + O$		3.0×10^{12}	0	25.0×10^3
$CO + O + M = CO_2 + M$		1.8×10^{19}	−1	2.0×10^3
$H_2 + O_2 = OH + OH$		1.7×10^{13}	0	24.7×10^3
$OH + H_2 = H_2O + H$		2.19×10^{13}	0	2.59×10^3
$OH + OH = O + H_2O$		5.75×10^{12}	0	0.393×10^3
$O + H_2 = H + OH$		1.74×10^{13}	0	4.75×10^3
$H + O_2 = O + OH$		2.24×10^{14}	0	8.45×10^3
$M + O + H = OH + M$		1.0×10^{16}	0	0
$M + O + O = O_2 + M$		9.38×10^{14}	0	0
$M + H + H = H_2 + M$		5.0×10^{15}	0	0
$M + H + OH = H_2O + M$		1.0×10^{17}	0	0
$O + N_2 = N + NO$		1.36×10^{14}	0	3.775×10^4
$N_2 + O_2 = N + NO_2$		2.7×10^{14}	−1	6.06×10^4
$N_2 + O_2 = NO + NO$		9.1×10^{24}	−2.5	6.46×10^4
$NO + NO = N + NO_2$		1.0×10^{10}	0	4.43×10^4
$NO + O = O_2 + N$		1.55×10^9	1	1.945×10^4
$M + NO = O + N + M$		2.27×10^{17}	−0.5	7.49×10^4
$M + NO_2 = O + NO + M$		1.1×10^{16}	0	3.30×10^4
$M + NO_2 = O_2 + N + M$		6.0×10^{14}	−1.5	5.26×10^4
$NO + O_2 = NO_2 + O$		1.0×10^{12}	0	2.29×10^4
$N + OH = NO + H$		4.0×10^{13}	0	0
$H + NO_2 = NO + OH$		3.0×10^{13}	0	0
$CO_2 + N = CO + NO$		2.0×10^{11}	−½	4.0×10^3
$CO + NO_2 = CO_2 + NO$		2.0×10^{11}	−½	2.5×10^3

[a] Reverse reaction rate k_r is obtained from k_f and the equilibrium constant K_c.

boundary conditions, a finite-difference computation of the mixing region external to the recirculation zone is carried out to the end of the recirculation region. This calculation defines the species mass fraction and temperature gradients along the dividing streamline, and these values are used to obtain the stirred reactor feed rates. A new stirred reactor computation is carried out using these feed rates, resulting in a new specification of the species mass fractions and temperature within the recirculation region, and the parabolic mixing computation is repeated. This procedure is continued until changes in the stirred reactor composition and temperature from computation to computation become small, typically 0.1%, at which point the coupling iteration has converged. The parabolic calculation is then carried out to the end of the combustion chamber, completing the solution.

As described in Ref. 1, the most critical of the model coefficients required for a modular model solution are the "skin friction" coefficient and the recirculation zone values of turbulent kinetic energy and its associated dissipation rate. For a given combustor, these coefficients can be adjusted by comparison of predicted and experimentally determined wall static pressure profiles at one operating condition. For all calculations reported herein, the "skin friction" coefficient was assumed to be 0.050; the recirculation region turbulent kinetic energy was taken to be $0.10(U_2)^2$; and the recirculation region dissipation rate was computed using the Kolmogorov hypothesis $\epsilon = 1.7k^{3/2}/l_K$, with an effective length scale l_K equal to the recirculation zone length.

Model Assessment: Entrainment Rate into Recirculation Region

The entrainment rate into the recirculation region is an important parameter in the overall combustor flowfield computation, and in the modular model this parameter is not specified, but is calculated as a part of the solution. Thus it is of considerable interest to compare the computed entrainment rate with experimental data. A variety of data for recirculation region entrainment rates was reviewed by Curran[7]

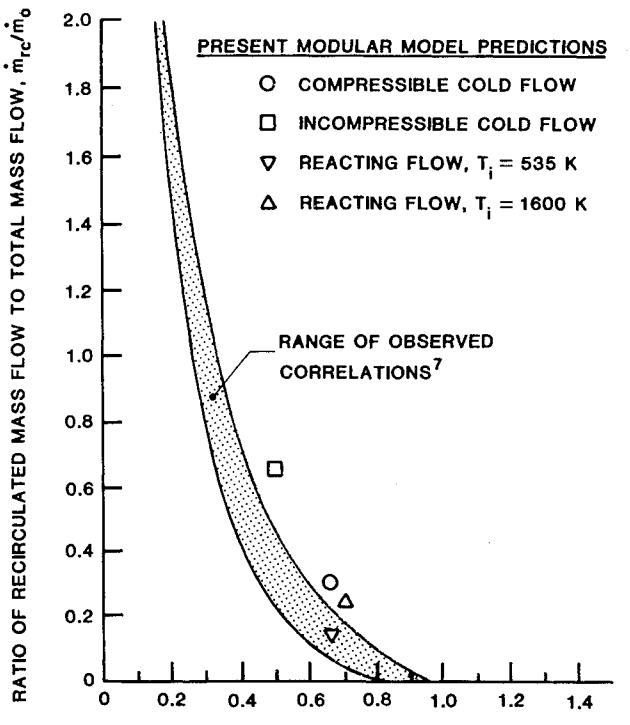

Fig. 3 Comparison of measured and predicted entrainment rates.

and the range of the observed correlations is shown in Fig. 3: These correlations are for both cold flow and hot flow. Also shown in Fig. 3 are the entrainment mass flux ratios predicted using the modular model in several different calculations, involving different area ratios for cold flow and reacting flow. Other results from many of these computations are described in Ref. 1. The range of correlations shown did not

include data from the investigations for which the calculations shown in Fig. 3 were made; nevertheless, the predictions show good agreement with the data correlations. Of particular significance is the fact that the predicted reduction of the entrainment rate with combustion compared to cold flow at the same area ratio is in agreement with the observations reported by Curran.[7] This represents an important result, both from the standpoint of validation of the modular model approach and because it suggests a more systematic study that can be pursued using the analytical model to examine a wider range of operating conditions than those on which the correlations were originally based.

Application of Modular Modeling for Ramjet Performance Diagnostics

One of the most important determinants of liquid fueled ramjet performance is the fuel distribution at the combustor entrance. For the sudden-expansion liquid fueled ramjet, the interaction between inlet fuel distribution and recirculation zone state is a further important consideration. A variety of observations have shown that for wall injection of the fuel, the recirculation zone equivalence ratio is generally more fuel-rich than the overall (global) equivalence ratio. This is demonstrated by the data of Schmotolocha and Economos,[8] which were obtained for three different inlet conditions and at two different locations of the fuel injection orifices upstream of the dump plane. Indeed, the measurements described in Ref. 8 indicate that for overall equivalence ratios greater than 0.2, the equivalence ratio in the recirculation region is always greater than unity. These data are shown in Fig. 4, in which the results of a modular model computation at two overall equivalence ratios are also shown. As was the case for the entrainment rate predictions, the agreement between the experimental results and the computation is reasonably good, with respect to both magnitude and trend.

In the experiments described in Ref. 8, plain orifice fuel injection was used. For plain orifices, fuel penetration characteristics are reasonably well documented, and an empirical penetration correlation was used to establish initial conditions for the computations used to obtain the results shown in Fig. 4. However, plain orifices are not widely used in ramjet design because of their poor turndown characteristics, which result in the need for several sets of orifices to obtain a wide operating range. The most commonly used fuel injector in ramjet applications is the poppet injector, which has a much broader turndown range than does a plain orifice. However, penetration characteristics from poppet injectors under ramjet operating conditions are not well documented. Indeed, there exists one investigation[9] of poppet (and other nozzle) penetration characteristics under ramjet operating conditions in which it was observed that the penetration from poppets is essentially nil. While other results indicate that penetration characteristics similar to orifice injection can be obtained using poppets,[10] it remains clear that the penetration characteristics of poppets are not as well known as for plain orifices.

At one operating condition, which involves a relatively high inlet temperature, poor ramjet combustor performance was observed in a recent development program: At this one condition, performance was considerably poorer than at other test conditions. The combustor utilized in the test program was an axisymmetric sudden expansion, with a combustor L/D_4 of 5 and a combustor to inlet area ratio A_4/A_2 of 2.0. Liquid fuel was injected from six wall orifices $0.87D_4$ upstream of the dump plane; no flameholders were used. Review of the available results suggested that fuel distribution effects were a possible cause of the observed low performance, and in particular that at the operating condition in question the fuel penetration from the wall-mounted fuel injectors may have been negligible. To investigate this possibility, and to study the effects of fuel distribution on combustor performance, a series of parametric modular model computations was carried out.

In the modular approach, fuel injection is modeled using an empirical correlation for penetration and a breakup time correlation. The latter correlation defines the downstream position at which the penetration is computed; from this point the fuel spray is assumed to vaporize at a rate given by a bulk spray vaporization correlation. After injection, the fuel is assumed to reside in an annular region at the position specified by the penetration correlation, and spreading of this annulus is computed using a turbulent mixing model. For the conditions of interest in the parametric study, vaporization occurs rapidly, so that the parameter to be varied was the fuel penetration height.

Figure 5 shows the predicted recirculation zone equivalence ratio as a function of fuel penetration height obtained from the parametric study. Of particular interest is the result for near-zero penetration height, $l/r_0 \simeq 0$. Under this condition, for a global equivalence ratio of unity, the predicted recirculation zone fuel/air ratio is extremely fuel-rich, with $\phi_{RZ} = 4.5$. This high value of equivalence ratio produces a substantially cooler recirculation region than would be obtained for conditions nearer stoichiometric, and this in turn leads to reduced flame propagation rates and lower overall combustion efficiency. Evaluation of the effect of the rich fuel/air ratio in the recirculation zone on overall performance

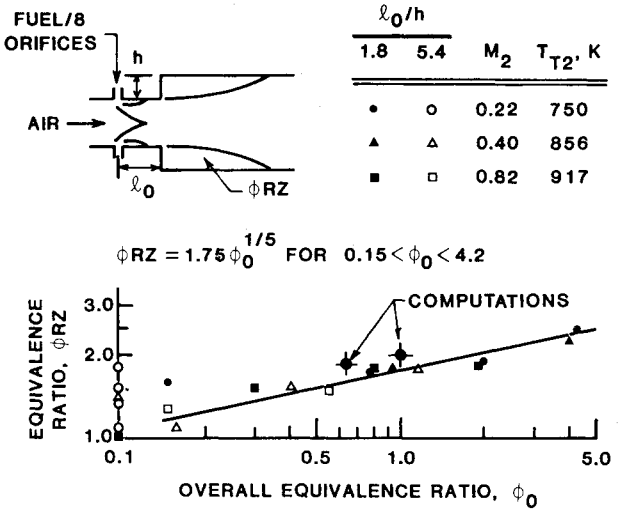

Fig. 4 Recirculation zone fuel concentration.

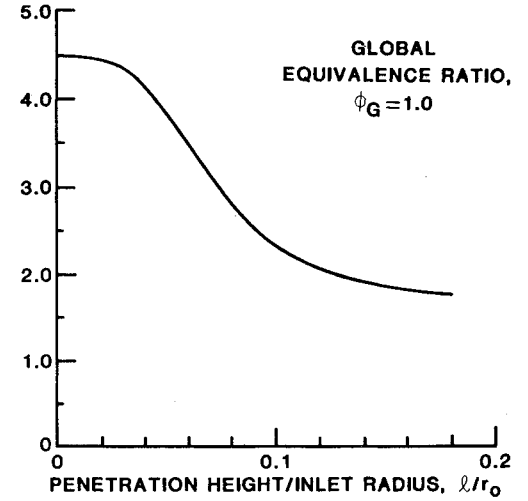

Fig. 5 Recirculation zone equivalence ratio as a function of penetration height.

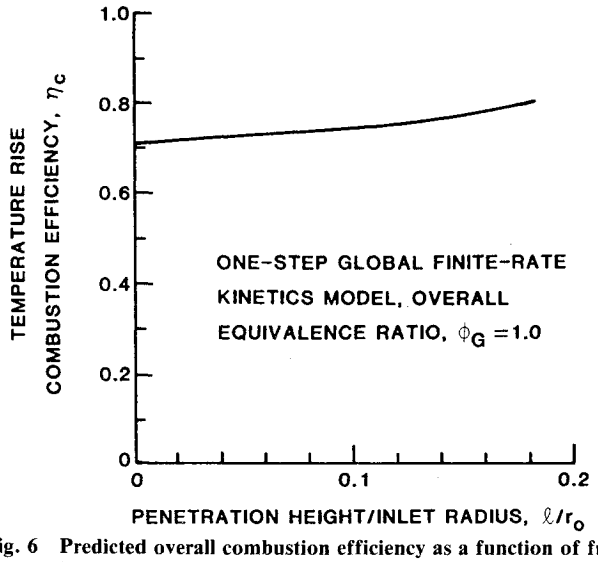

Fig. 6 Predicted overall combustion efficiency as a function of fuel penetration height.

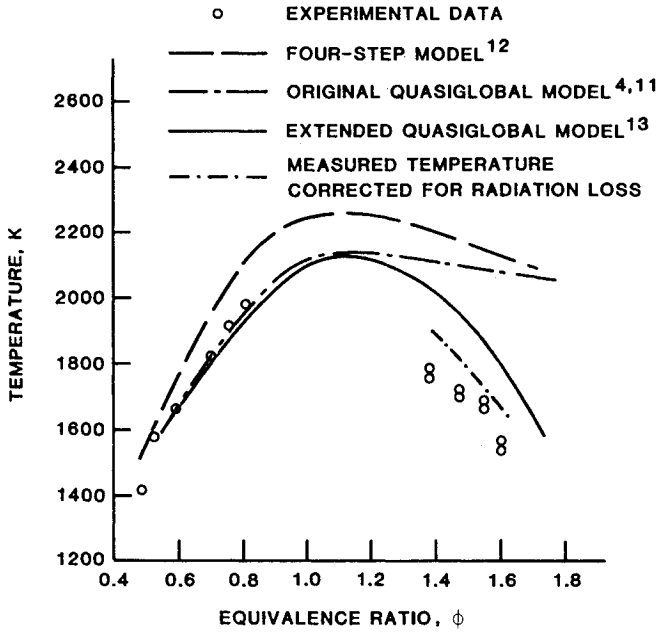

Fig. 7 Iso-octane combustion as measured in jet-stirred combustor and as predicted using well-stirred reactor formulation.

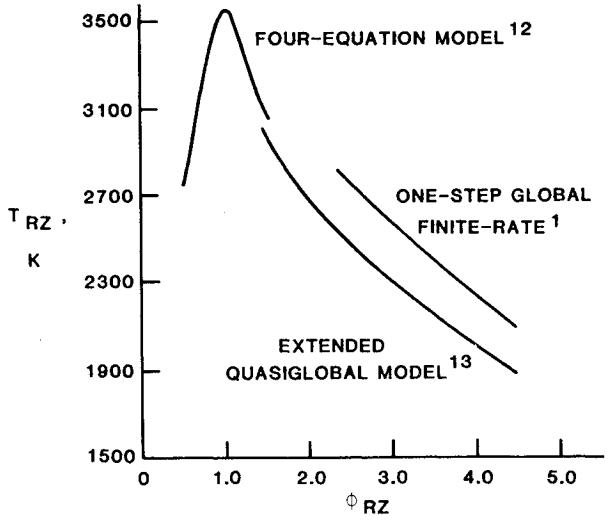

Fig. 8 Combustor recirculation zone temperatures computed using different chemistry models.

is, however, complicated by difficulties that are encountered in modeling chemical kinetics in very fuel-rich regions.

There is no currently available finite-rate chemical kinetics model which can provide adequate results for complex hydrocarbon fuels under fuel-rich conditions, at temperatures at which the effects of dissociation manifest themselves. The model used for the computations described in this paper includes as options either a one-step finite-rate kinetics formulation[1] or the multistep quasiglobal approach.[4,11] With the one-step model, the products of combustion are the fully reacted species H_2O and CO_2, so that the effects of dissociation are ignored; the overall reaction rate is underpredicted also. The quasiglobal model used in the modular formulation is valid for complex hydrocarbon fuels and includes the effects of dissociation, but is not appropriate for equivalence ratios much above stoichiometric. Other kinetics models have been proposed for fuel-rich conditions, such as the four-step model of Dryer and Glassman,[12] but this approach ignores dissociation effects. Thus it is difficult to obtain reliable estimates for the chemical kinetic rates that pertain in combustors in which significant regions of the flowfield are highly fuel-rich.

This difficulty is reflected in the performance results shown in Fig. 6. While the trend of combustion efficiency as a function of fuel penetration distance obtained through the use of the one-step global kinetics model is as expected, the magnitude of the overall change is relatively small and probably incorrect. The reason that the magnitude of these results can be expected to be incorrect is that the global finite-rate model can be expected to significantly overpredict the recirculation zone temperature for fuel-rich conditions, since the only effect of fuel-rich operation that this model recognizes is a dilution of the products of combustion with excess fuel for $\phi \gg 1$. With this model, the reaction rate is linear with respect to fuel concentration, whereas evidence exists that for fuel-rich conditions reaction rates do not continue to increase with fuel concentration, and, as noted earlier, dissociation effects are also ignored. Nevertheless, these results indicate that for the conditions considered, low values of fuel penetration distance are directly coupled to reductions in overall combustor performance. Since further development testing using fuel injection schemes designed to increase fuel penetration resulted in substantial performance improvements, it can be considered that the trends demonstrated by this modeling have been experimentally verified.

Modifications to the Modular Formulation

In the descriptions of the modular approach to the development of combustor models outlined in Refs. 1-3 and 6, it has been stressed that one of the features of the modular approach is that each of the elements involved in the overall combustor model can be independently developed. Just such an approach is being followed: the extension of the quasiglobal model to fuel-rich conditions is being explored using the well-stirred reactor element of the model. One result of this work is shown in Fig. 7, on which predictions using several different kinetics models are compared to measured temperature data obtained in a laboratory well-stirred reactor burning toluene under both fuel-lean and fuel-rich conditions. All of these results are for the same stirred reactor residence time. For fuel-rich conditions, Fig. 7 shows that the extended quasiglobal model substantially improves the stirred reactor temperature prediction as compared to either the original quasiglobal formulation[4,11] or the four-step model.[12]

Although the extended quasiglobal formulation has not yet been fully developed, an indication of the effect of using this approach in a combustor calculation is demonstrated by Fig. 8, which shows recirculation zone temperatures for the conditions of the preceding section, computed using the four-step model,[12] the one-step model,[1] and the extended quasiglobal formulation. While these results are provisional

in that the extended quasiglobal model has not at this point been verified for ramjet fuels or operating conditions, they indicate a significant effect on recirculation zone temperature: The temperature predicted using the extended quasiglobal model is some 300 K lower than that obtained from the one-step model. This difference, coupled with the radically different species distributions obtained from the two models, can be expected to exert a significant influence on predicted flame propagation rates.

Conclusions

A comparison of modular model predictions with available data shows that the model is capable of predicting both the entrainment rate into sudden-expansion combustor recirculation regions and the overall fuel/air ratio in these regions. Both of these parameters are crucial to investigations of flame stability in a liquid fueled sudden-expansion combustor. An application of the approach in the interpretation of ramjet combustor test data has also been demonstrated: This demonstration shows that the model provides a means of verifying suspected causes of combustor performance deficiencies. The inadequacy of current chemical kinetics models under very fuel-rich conditions in circumstances under which the effects of dissociation are apparent provides a current limitation on the use of the modular model approach. However, related chemical kinetic model development work which can remove this limitation has been described.

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References

[1] Edelman, R.B., Harsha, P.T., and Schmotolocha, S.N., "Modeling Techniques for the Analysis of Ramjet Combustion Processes," *AIAA Journal,* Vol. 19, May 1981, pp. 601-609.

[2] Harsha, P.T. and Edelman, R.B., "AFOSR Interim Scientific Report: Mixing and Combustion in High Speed Air Flows," Science Applications, Inc., Chatsworth, Calif., AFOSR TR 79-0912, April 1979.

[3] Harsha, P.T. and Edelman, R.B., "Application of Modular Modeling to Ramjet Performance Prediction," AIAA Paper 78-944, July 1978.

[4] Edelman, R.B. and Fortune, O., "A Quasi-Global Chemical Kinetic Model for the Finite-Rate Combustion of Hydrocarbon Fuels," AIAA Paper 69-86, Jan. 1969.

[5] Launder, B.E., Morse, A., Rodi, W., and Spalding, D.B., "Prediction of Free Shear Flows—A Comparison of the Performance of Six Turbulence Models," *Free Turbulent Shear Flows, Vol. I, Conference Proceedings,* NASA SP-321, 1973, pp. 463-519.

[6] Harsha, P.T. and Edelman, R.B., "Mixing and Combustion in High Speed Air Flows," Science Applications, Inc., Chatsworth, Calif., AFOSR TR 80-1005, July 1980.

[7] Curran, E.T., "An Investigation of Flame Stability in a Coaxial Dump Combustor," Ph.D. Thesis, Air Force Institute of Technology, Wright-Patterson AFB, Ohio, 1979.

[8] Schmotolocha, S.N. and Economos, C., "An Experimental Combustion and Flame Stabilization Study of Dump Burners," General Applied Science Laboratories, Westbury, N.Y., AFOSR TR 75-1446, Sept. 1975.

[9] Rosfjord, T.J., "Experimental Investigation of Fuel Sprays Formed by Ramburner Injectors," Paper presented at the 1979 JANNAF Propulsion Meeting, Vol. 2, CPIA Publication 300, 1979, pp. 585-607.

[10] Pelmas, R.J. et al., "Integral Boost Ramburner Technology for Volume-Limited Missiles," Air Force Aero Propulsion Laboratories, Wright-Patterson AFB, Ohio, AFAPL-TR-73-55, Vol. I, July 1973.

[11] Edelman, R.B. and Harsha, P.T., "Laminar and Turbulent Gas Dynamics in Combustors—Current Status," *Progress in Energy and Combustion Science,* Vol. 4, No. 1, 1978, pp. 1-62.

[12] Hautman, D.J., Dryer, F.L., Schug, K.P., and Glassman, I., "A Multistep Overall Kinetic Mechanism for the Oxidation of Hydrocarbons," *Combustion Science and Technology,* Vol. 25, Nos. 5 and 6, 1981, pp. 219-225.