Three-Dimensional, Primitive-Variable Model for Solid-Fuel Ramjet Combustion

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A three-dimensional computer code has been developed for the solid-fuel ramjet combustion process. The code is an adaptation of the Garrett gas turbine combustor code, which includes finite-rate chemical kinetics and has been used to predict the combustion behavior for axial inlet, side-dump inlet, and bypass configurations. The model shows that inlet swirl can be used to both increase the fuel regression rate and improve fuel utilization. Significant variations in the fuel regression rate and regression uniformity were also predicted as the air injection location and dump inlet size were varied. Model predictions were in qualitative agreement with the limited existing experimental data. The model can provide valuable input about the sensitivity of fuel utilization to design changes. However, much additional model validation work is required before it can be expected to provide quantitative performance predictions.

Nomenclature

A = constant in regression rate, Eq. (7)
B = blowing parameter
C_p = specific heat at constant pressure
D = fuel grain diameter
E = activation energy
h = enthalpy, inlet step height
h_f^0 = heat of formation
k = turbulence kinetic energy
$\dot{m}$ = mass flow rate
$\bar{M}$ = average molecular weight
m_i = mass fraction of species i
p,P = pressure
$\dot{q}''$ = heat-transfer flux
r = radial distance
$\dot{r}$ = fuel regression rate
R = universal gas content
R_i = reaction rate of species i
T = temperature
u = axial velocity
v = radial velocity
w = tangential velocity
x = axial distance
Γ_i = effective transport coefficient of species $i = \mu/\sigma$
δ = incremental distance from wall
ϵ = turbulence dissipation rate
θ = circumferential direction
μ = effective viscosity
ρ = density
σ_i = Prandt or Schmidt number for species i
ϕ = mixture fraction (mass fraction of total fuel)

Subscripts

a = air
c = chamber
CO = carbon monoxide
CO_2 = carbon dioxide
CH = intermediate hydrocarbon
f = solid fuel
fu = unburned fuel vapor
g = within the fuel grain
H_2 = hydrogen
H_2O = water
i = inlet
O_2 = oxygen
p = near wall node point, port
T_w = wall temperature
rad = radiation
w = fuel wall

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Introduction

THE solid-fuel ramjet (SFRJ) most often consists of a solid-fuel grain that provides the walls for the combustion chamber. A sudden expansion at the air inlet (either axial or side-dump) can be used to provide flame stabilization. Downstream of the flow reattachment a turbulent boundary layer develops and includes a diffusion-controlled flame between the fuel-rich zone near the wall and the oxygen-rich central core. Due to that diffusion flame, heat is transferred by convection and radiation to the solid surface, causing vaporization of the fuel.

At the Naval Postgraduate School (NPS) both mathematical modeling[1-4] and experimental efforts[5-10] have been conducted to determine the effect of design and operational variables on the obtainable performance. Many additional SFRJ investigations have been conducted throughout the world, with Chemical Systems Division, United Technologies (CSD)[11,12] being the dominant developer within the United States.

The SFRJ combustor modeling conducted at CSD[11,12] has centered on the development of empirical correlations for average fuel regression rate and combustion efficiency as influenced by geometry and operating environment. These correlations are a necessity in any development effort because they allow for rapid calculations of expected performance in tradeoff studies. However, these correlations were not derived for, and cannot be expected to predict fuel/combustion behavior in, significantly new geometries, especially those involving significant three-dimensional flow environments.

Computer modeling of the SFRJ combustion process is directed at the need for an additional engineering tool, one that can be used to qualitatively predict the effects on fuel utilization and the internal flowfield by the new complex air injection and combustor geometries which are needed to improve fuel loading, combustion efficiency, etc. Computer model simulation of the SFRJ combustion process at NPS has evolved from an original stream-function vorticity formulation[1] to a primitive-variable (pressure, velocity) model that includes an aft mixing chamber.[3] In these earlier axisymmetric models, radiative heat transfer to the fuel surface was not included. Radiation can be significant in the SFRJ, depending upon the fuel composition. Most of the radiation results from

the presence of carbon within the flame zone with lesser amounts from water vapor, carbon dioxide, and carbon monoxide. Formulation of the effects of radiation on the solid-fuel regression rate were developed originally for the hybrid rocket.[13] This type of analysis is used in the present CSD SFRJ model.[11,12] A simplified radiation model[4] was also incorporated into the primitive-variable model and resulted in improved prediction of the fuel regression rate profile for fuels that produce significant unburned free carbon. The primitive-variable codes were based on the Champion 2/E/FIX computer program developed by Pun and Spalding.[14] The Champion code is two-dimensional and, therefore, could not be used to model two important SFRJ geometries, side-dump and bypass. The side-dump configuration has air injected through the side of the fuel gain and the dome region is constructed of fuel. The bypass configuration ducts a portion (typically 50%) of the total airflow into an aft mixing chamber. A full three-dimensional (3D) model is needed to predict the flowfield in these configurations.

The side-dump configuration is a very difficult one to develop/optimize using only experimental data. There is a complex interaction between the location/size of the inlet dump, the length of the dome region upstream of the dump, and the resulting fuel regression rate pattern. Very little regression rate data has been generated to date for the side-dump geometry. However, several general observations can be made. Swirling the inlet flow can increase and smoothout[11] the downstream fuel regression rate pattern. Regression rates within the dome region (upstream of the dump) can increase or decrease, depending upon the dome length, number of inlets, and amount of swirl. Three-dimensional models are, in this case, a necessity in the combustor development process.

Three-dimensional, elliptic, primitive-variable codes have been used for several years to model combustion processes.[15] Most efforts have been extensions of the earlier Champion 2D code.[14] The best documented and most readily available 3D code has been developed to model gas turbine combustors by Mongia et al. at the Garrett Turbine Engine Company.[16-18] This code is an extension of the Champion code. Reference 18 presents an excellent summary of the state-of-the-art of 3D, turbulent combustion modeling. Both mathematical modeling limitations and experimental validations are discussed. The authors have pointed out the model deficiencies related to the turbulence and chemistry submodels, the numerical solution method, and the need for accurate specification of boundary conditions.

The purpose of the present investigation was to adapt the Garrett 3D code to the specific geometry and flow environment of the solid-fuel ramjet. Such a 3D SFRJ code is needed as a basic design/development tool for estimating the effects of changes in combustor geometry, fuel configuration, and the method of air injection on the fuel regression pattern and on the combustion flowfield.

Model Overview

The Garrett/AiResearch Model is 3D, elliptic, for steady, subsonic flow and includes finite-rate chemical kinetics. The dependent variables are u, v, w, h, k, ϵ, ϕ, m_{fu}, m_{CH}, m_{H_2} and m_{CO}. In addition, if radiation is included (a six-flux model), three radiation flux vectors are calculated. Soot emissions can be calculated if desired. Liquid spray calculations can also be made, but were not necessary in the SFRJ model. The turbulence model is the same as used in the Champion program, namely, the modified two-equation ($k-\epsilon$) model of Jones, Launder, and Spalding.[19,20]

Hydrocarbon combustion is considered to be a four-step process as follows:

$$C_xH_y \rightarrow C_xH_{y-2} + H_2 \tag{1}$$

$$C_xH_{y-2} + \frac{x}{2}O_2 \rightarrow xCO + \frac{y-2}{2}H_2 \tag{2}$$

$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2 \tag{3}$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O \tag{4}$$

Arrhenius rate expressions are included for each of the above reactions. In the Garrett code, the chemical kinetics rate expressions are compared to rate expressions based on an eddy-breakup model for every control volume in the solution grid. The latter expressions attempt to account for the effects of turbulence intensity and scale and species concentration on the consumption rate of a particular reactant. The rate of oxidation at each solution point is taken as the minimum of the kinetics and eddy-breakup rates. The two-part boundary layer (divided by $y^+ = 11.5$) used in the Champion code is also employed. Details of the computer program, the differential equations, and the line-by-line, finite difference solution procedure are presented in Refs. 16 and 17.

Model Modifications and Solution Procedures

The major modifications required of the Garrett/AiResearch model were the inclusion of geometric changes and of a fuel wall, adjacent to which finite-rate, gas-phase chemical kinetics could occur. The geometric changes required to model the SFRJ configurations (Fig. 1) were readily incorporated by selectively locating and sizing the inlet dome, "inclined walls," cooling slots, and radial injection holes that are provided within the input data. Several additional variables and subroutines were necessary to include the "blowing-wall" fuel surface effects as discussed below. In addition, fuel property subroutines were changed to reflect the properties of Plexiglas (PMM) and HTPB, the two solid fuels used in the present study.

The governing equations on the boundary[21] for unity Lewis number are

Energy:

$$\dot{q}''_{rad} = (\rho v)_w (h_w - h_f) + \Gamma_{h_w} \left(\frac{\partial h}{\partial r}\right)_w \tag{5}$$

$\dot{q}''_{rad}$ can be calculated within the existing model but was neglected in the present investigation.

Species:

$$R_{i_w} = \Gamma_{i_w} \left(\frac{\partial m_i}{\partial r}\right)_w + (\rho v)_w (m_{i_w} - m_{i_g}) \tag{6}$$

The values of R_{i_w} were calculated in the same manner as for the internal nodes.

It was assumed that the fuel regression rate could be represented in an Arrhenius format,[22]

$$\rho_f \dot{r} = (\rho v)_w = A \rho_f e^{-E/RT_w} \tag{7}$$

Using the Couette flow approximation for the boundary-layer behavior with mass transfer[1,21]

$$\Gamma = \Gamma_{B=0} \frac{\ell n(1+B)}{B} \tag{8}$$

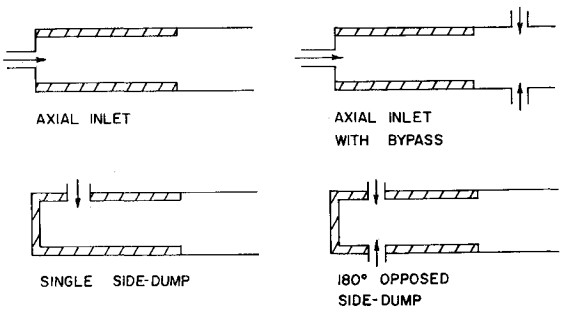

Fig. 1 Solid-fuel ramjet geometries in model.

where B can be evaluated from the enthalpy as

$$B=\frac{hp-h_w}{h_w-h_{fg}-[\dot{q}''_{\rm rad}/(\rho v)_w]} \tag{9}$$

The enthalpy can be expressed as

$$h_w=\sum_i m_i\left(h^0_{fi}+\int_{T_{\rm ref}}^{T_w} C_{po}\,dT\right) \tag{10}$$

The solution procedure for the boundary conditions on the fuel wall was as follows:

1) Estimate T_w and B.
2) Calculate $(\rho v)_w$ from Eq. (7).
3) Calculate Γ_{iw} and Γ_{hw} from Eq. (8).
4) Calculate m_{iw} for all species from Eq. (6).
5) Calculate the other species ($m_{\rm H_2O}$, $m_{\rm O_2}$, $m_{\rm CO_2}$, $m_{\rm N_2}$) from species conservation equations.
6) Calculate h_w from Eq. (10).
7) Calculate B from Eq. (9) with $\dot{q}''_{\rm rad}=0$.

Iterate steps 3-7 until B converges.

8) Calculate $(\rho v)_w$ from Eq. (5).
9) Calculate T_w from Eq. (7).

Iterate steps 2-8 until $(\rho v)_w$ converges.

10) Calculate ρ_w from $\rho_w=P/[T(R/\bar{M})]$.
11) Calculate v_w from $(\rho v)_w/\rho_w$.

It was found, as previously noted by Netzer[1] and Stevenson and Netzer,[3] that the near-wall turbulence dissipation had to be increased on the step face ($\epsilon_p=k_p^{3/2}/0.4$). Also, as discussed by Stevenson and Netzer,[3] the grid spacing adjacent to the fuel surface had to be maintained slightly less than that required for $y^+=11.5$ in order to obtain temperature distributions in qualitative agreement with experimental data. When the wall shear stress is calculated using a grid point within the laminar sublayer ($y_p{}^+<11$), a linear velocity profile is assumed. However, the source terms for k and ϵ imply that $\mu_{\rm eff}/\mu_{\rm laminar}$ is much greater than unity. This precludes $y_p{}^+$ from being significantly less than 11.5.

To obtain convergence, it was necessary to input initial conditions that were in qualitative agreement with the final solution. In the Garrett code, for example, the initial temperature distribution is based upon an assumed "realistic" initial fuel distribution. When modeling the SFRJ, it was necessary to specify the initial conditions for fuel mass fraction and temperature to be decreasing with increasing distance from the wall. Otherwise, rapid divergence of the solution occurred. Under-relaxation was required, typically between 0.1 and 0.5. Turbulence parameters (k and ϵ) and gas density calculations generally required the lowest values for the relaxation parameters. A $40\times33\times9$ (x,r,θ) grid was used in the present study.

Results and Discussion

Four geometries were investigated (Fig. 1): axisymmetric with axial inlet, bypass with axial upstream inlet, single side-dump, and dual side-dump. All cases included an aft mixing chamber. For the axisymmetric, axial inlet geometry, the predicted reattachment "points" (where u near the wall was interpolated to zero) are shown in Fig. 2. The predicted reattachment "points" were in good agreement with the maximum heat-transfer locations measured by Krall and Sparrow,[23] but upstream from those measured by Phaneuf and Netzer[6] in nonreacting flow with wall mass addition. In general, the flow reattachment location moves upstream slightly when wall mass addition is present.[6] The model predicts a reattachment length between approximately 5.5 and 7.0 inlet step heights. Experimental data[1] generally indicates reattachment lengths between 7.0 and 8.0 inlet step heights. This prediction of shorter reattachment lengths was also observed by Mongia et al.[18] and was attributed (possibly) to the use of wall functions in the model.

Normalized regression rate profiles are shown in Fig. 3. The experimentally measured profiles for PMM fuel were very sensitive to inlet turbulence/distortion. The 3D code (with finite rate kinetics) predicted results very nearly identical to the mixing limited, 2D code,[3] i.e., the maximum regression rate was predicted to occur upstream of the experimentally measured point. This was due to the short reattachment locations discussed above. The average regression rate was in good agreement with experiment. As discussed above, the computer code automatically takes the slowest process (kinetics or turbulent mixing) to be rate controlling at each solution point within the grid. The agreement with the 2D, mixing limited code predictions indicates that most of the combustion process was mixing limited in the present calculations for combustion at approximately 4 atm pressure. However, at high-altitude conditions, kinetics may become dominant in major portions of the combustor. The present scheme appears warranted for general application to all SFRJ operating environments, although it is more time consuming than necessary for calculations at higher pressures.

As discussed above, boundary conditions on the inlet step face in the SFRJ geometry have a strong influence on whether or not the predicted temperature and fuel mass fraction distributions are in qualitative agreement with experimental data. Small changes in the fuel regression rate expression [Eq. (7)] also can have large effects on the fuel regression rate and, therefore, on the location of the diffusion flame located within the developing boundary layer. This sensitivity of the predictions for the entire combustor to the wall boundary conditions is unfortunate and apparently results from the distributed nature of the fuel injection along the entire length of the combustor wall. Upstream effects accumulate to effect downstream predictions.

Examples of typical radial profiles calculated for u, $m_{\rm O_2}$, $m_{\rm N_2}$, and T near the grain exit are shown in Fig. 4. The effects

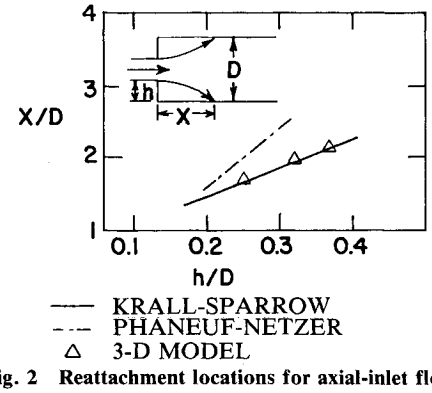

Fig. 2 Reattachment locations for axial-inlet flow.

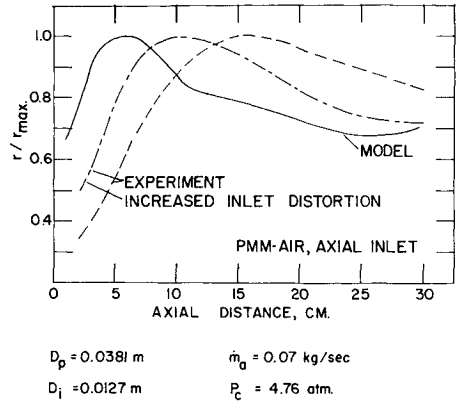

Fig. 3 Fuel regression rate profiles for axial-inlet flow.

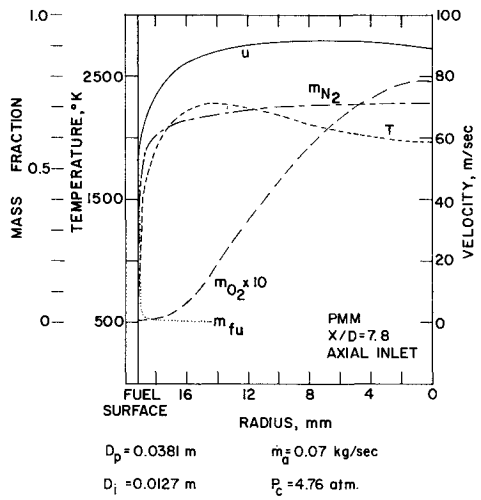

Fig. 4 Predicted radial profiles for gas properties near the grain exit, axial-inlet flow.

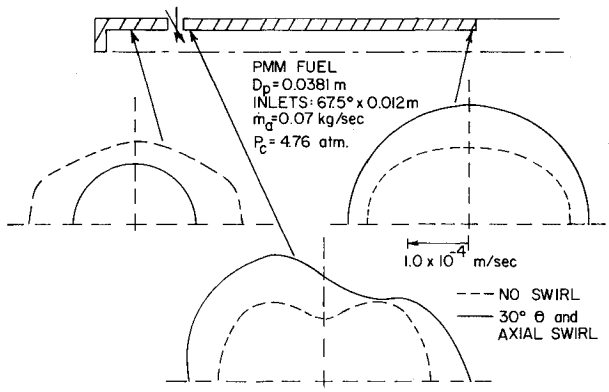

Fig. 5 Effects of inlet swirl on fuel regression rate profiles, 180 deg opposed side-dumps.

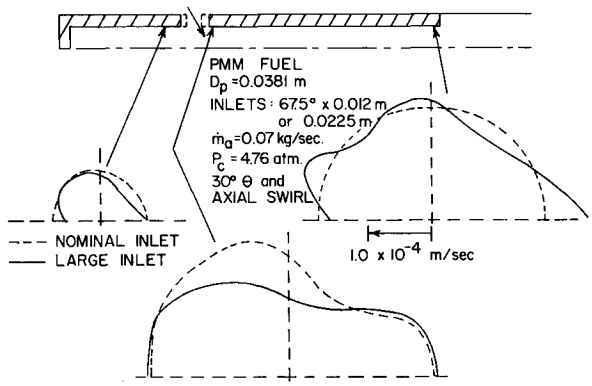

Fig. 6 Effects of inlet area on fuel regression rate profiles, 180 deg opposed side-dumps with inlet swirl.

of including finite rate kinetics and/or the injection of O_2 that occurs into the boundary layer near the reattachment zone are readily apparent; a broad zone of high temperature near the maximum value and finite concentrations of oxygen below the flame. Figure 5 shows the predicted regression rate results with two, 180 deg opposed side-dumps, with and without inlet air swirl. Inlet swirl is introduced into the model through specification of the u, v, and w components of the air inlet velocity. In the present example, the inlet velocity vector was oriented 30 deg from the normal vector ($u = w = 0$) in both the axial (u) and tangential (w) directions. The effects of inlet swirl on this particular geometry are readily apparent. Inlet swirl significantly decreased the regression rates in the dome, but significantly increased the rates downstream. Regression rate uniformity was also significantly improved except adjacent to the inlet dump.

Figure 6 shows the results of increasing the inlet dump area in a combustor with a long dome length and inlet swirl. Increasing the inlet area in this case resulted in greatly increased nonuniformity in the fuel regression rate. Comparison of Figs. 5 and 6 shows the predicted effects of dome length on the regression rate pattern when inlet swirl is used. Lengthening the dome (Fig. 6, nominal inlet) above the reference value (Fig. 5, swirl) reduced head-end fuel regression rates without major effects in the downstream regions.

Conclusions

The model predictions show that significant variations in fuel regression rate (both circumferentially and axially) are caused by the manner in which the air is injected into the fuel grain. In general, inlet swirl can be used to both increase the fuel regression rate downstream of a side-dump inlet and to improve fuel utilization. The effects of inlet location and size on the regression rate behavior are difficult to estimate a priori for a specific set of test conditions. The model must be used to predict the expected results. Much additional work is required in order to validate the predictions of the three-dimensional SFRJ model. However, the ability to examine the qualitative effects of inlet air location and flow characteristics on the fuel regression rate pattern (and the combustion efficiency, etc.) has provided a valuable engineering design tool and a needed improvement to the earlier two-dimensional model.

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