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COMBUSTION IN HIGH SPEED

AIR FLOWS

FINAL REPORT

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1. RESEARCH OBJECTIVES AND SUMMARY

The results described in this report have been obtained from work whose overall objective is the analysis of reacting multiphase flows in advanced air-breathing propulsion systems. This work involves the formulation and evaluation of new theoretical descriptions of multiphase turbulent mixing and chemical kinetic phenomena in subsonic and supersonic air flows, and the generation of new experimental data on these phenomena. The specific objectives of this research may be described as follows:

- (a) <u>Spray Modeling</u>; This task area involves the development of analytical models of the phenomena occurring in the multiphase turbulent reacting flows involved in spray flame evolution. The model is to include the effects of hetergeneous and homogeneous finite rate chemical reaction, turbulent transport, and velocity and temperature nonequilibrium between the droplets and gas phase. Both liquid fuels and slurries are to be considered. The analytical modeling work is to be supplemented with experimental studies of spray injector characteristics and spray flame structure for both ramjet and gas turbine applications.
- (b) Modeling of Boron Combustion Processes; In this task area advanced analytical models of the combustion of boron particles are to be developed. A survey of the existing boron kinetics literature is to be performed to provide the data base for the development of advanced boron kinetics models. This survey leads to the definition of an advanced model for boron particle combustion, to be incorporated in modular models of slurry combustion process in ramjet. Required boron kinetics data are also to be defined.
- (c) <u>Modeling of Ramjet Combustion Processes</u>; The modular modeling approach to the analytical characterization of high speed combustion processes is to be further refined and developed, and applied to the analysis of results generated from experiments relevant to high speed combustion

processes. Model refinements including the advanced quasiglobal chemical kinetics model for the characterization of fuel-rich combustion of complex hydrocarbon fuels and the spray model formulations developed under item (a) above are to be incorporated. This modeling work will also emphasize slurry fuels, particularly boron slurries. Of specific importance in this area is the experimental data on gas-phase, liquid-phase, and slurry-fuel combustion phenomena being obtained at the Naval Weapons Center under a joint AFOSR/NWC sponsored program. Also of importance in this area is the continued development of unified elliptic computational techniques for modeling ramjet combustion processes.

(d) Modeling of the Ducted Rocket Combustion Process. This task area involves the formulation and development of a modular model for the ducted rocket combustor. This model is to be based on a delineation of flow characteristic regions obtained through the use of three-dimensional elliptic aerodynamic caculations, and is to be used to develop a broad base of new and fundamental information on three-dimensional multi-stream interaction in reacting ducted flows.

Work carried out to meet these objectives during the contract period resulted in a number of significant accomplishments. In summary, these accomplishments include:

(a) <u>Development of a Comprehensive Spray Flame Model</u>: A spray flame model was completed which includes sub-models for two-phase transport and diffusion, hetero-geneous and homogeneous combustion kinetics, turbulent mixing, gas-phase radiation, and buoyancy effects. Based on the assumption of near dynamic equilibrium, this approach allows a detailed computation of the evolution of the droplet size distribution throughout the flame, and incorporates the advanced quasiglobal

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kinetics model to accurately account for gas-phase hydrocarbon combustion processes in fuel-rich regions of the flame. Utilization of the model to predict spray flame development has shown the necessity of incorporating accurate representations of physical processes which control the flame development, including those mechanisms which occur on a droplet scale but also including gas-phase phenomena involving finite-rate kinetics, thermal radiation, and, for the flowfield considered, buoyancy. The computer model that has been developed from this work provides a generalized framework for the development and testing, in conjunction with key experimental data, of physically perceptive models of the many mechanisms involved in spray combustion.

(b) Development of an Accurate Boron Combustion Model: Based on the results of a survey of boron combustion modeling, an exiting model in which both diffusion and chemical kinetics mechanisms are implemented was selected for further development. The model is based on a clean-particle assumption - it is assumed that no B_2O_3 layer is present. Since particle consumption at a significant rate can only occur for clean particles, this approach allows examination of the effects of kinetics limitations on boron consumption rate. The model, coupling finite rate oxidation kinetics and diffusional mechanisms, shows excellent agreement with experimental data for boron particle burn time as a function of particle size, temperature and pressure. Further, the model indicates that kinetics effects enter over the entire size range of interest. The model results also predict quenching for certain combinations of particle size, environment pressure and temperature, and environment 0, concentration. These results indicate a critical balance between heat generation and heat

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loss on the particle scale, indicating that the coupling of fluid dynamics and particle cloud processes is of fundamental importance in the combustion of boron in practical systems.

(c) Modeling of Ramjet Combustion Processes: Under this program, a detailed modular model for sudden-expansion ramjet combustor performance evaluation was completed. This model combines state-of-the-art representations of the turbulent mixing and chemical kinetics rate processes with submodels for the fuel injection, vaporization and mixing phenomena in the combustor inlet. It is founded on the use of a perfectly-stirred reactor model to represent largescale recirculation regions in the combustor and, in particular, the flame stabilization characteristics of these regions. A variety of computations have been carried out using this approach, under this and other Air Force- and Navy- sponsored programs, to analyze and interpret experimental data obtained using a variety of sudden-expansion ramjet configurations. Results of this work have demonstrated the role of the sudden-expansion recirculation regions in flame stabilization at lower Mach numbers, that performance fall-off at high overall fuel-air ratios at moderate flight Mach numbers can be directly related to the effects of fuel-rich combustion in large regions of the combustor flowfield, and that a desirable fuel distribution at high Mach number is considerably different from that which is desirable at lower Mach numbers. All of these results provide a critical input to the analysis and interpretation of ramjet performance data.

In addition to the modular approach, development of elliptic Navier-Stokes solution techniques has also continued. This work has centered on the examination of turbulence models, and has shown that

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the algebraic stress modeling approach can provide a potentially more valid description of turbulent mixing in combustor flowfields. The increased generality of the algebraic stress modeling approach is of particular importance in swirling flows where large-scale nonisotropy of the apparent viscosity is evident. At the same time, this work has demonstrated that for many combustors of interest, for example, axisymmetric sudden expansions with area ratios of four or more, inertia effects dominate in much of the flow, thus reducing the effect of choice of turbulence model on the overall flowfield prediction.

(d) <u>Ducted Rocket Model Development</u>: Work in this area focused on the examination of different techniques for the prediction of ducted rocket flowfields and performance. Aerodynamic flowfield predictions were carried out for a representative combustor flowfield, but without simulation of the gas generator exhaust. Limited modular model evaluation of ducted rocket performance characteristics was also accomplished. Examination of available modeling approaches applicable to the ducted rocket showed that none examined accounted for the mixing and shock interaction effects of a highly underexpanded gas gnerator fuel jet. The existence of this key feature of the flowfield, which may well dominate the overall flow structure, should be included in any ducted rocket modelling approach.

Although as noted in the proceeding paragraphs, there have been considerable advances made in each of the research areas considered under this project, profitable research work can still be carried out in each of these areas. In the following paragraphs the research recommendations that result from the work already done are outlined:

(a) <u>Spray Modeling</u>: Two avenues of approach can be taken in further spray modeling work. With the existing model,

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experiments can be designed which will closely approximate the model assumption, so that direct comparisons of the various aspects of the model predictions which data can be made. In this way, each of the submodels incorporated in the overall spray model can be examined, to provide information on, for example, the effects and importance of droplet interactions, droplet/turbulence, combustion/turbulence and radiation/turbulence interactions, and the effects of different diffusion rates for droplet and gas phase. This would then provide a wealth of further data on droplet transport and spray combustion phenomena in a regime where the droplet and gas phase motions are nearly in equilibrium. The second avenue of investigation involves the relaxation of the near equilibrium hypothesis. Within the context of the present model an Eulerian formulation for droplet transport can be constructed, and a Lagrangian formulation can also be defined. Note that by carrying out such an analysis for a flowfield which in general satisfies the boundary layer assumptions, as in the present spray flame formulation, many of the numerical problems inherent in elliptic Navier-Stokes solution techniques can be avoided, an important consideration in establishing an understanding of the phenomena while maintaining relevance to airbreathing propulsion systems.

(b) Boron Combustion Modeling: Work accomplished to date shows the importance of incorporating both diffusional and kinetics mechanisms in developing an accurate model for particle-scale boron combustion processes. There are several areas of research and model improvement that this work suggest. Extension of the model to include the effects of the existence of an oxide layer is clearly a critical need with respect to the practical use of the existing approach. At the same time, there are several other areas which require continued research. For example, the potential importance of suboxide formation and disposal is at the present unclear and requires further investigation, while more mechanistic models of B-O, B-O-H, and B-O-H-C kinetics

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are also needed. Further, finite rate condensation of B_2O_3 is important in the overall heat release process, and itself represents an important area of continued research related to problems of boron combustion.

- (c) Modeling of Ramjet Combustion Processes: Work carried out under this and other programs has shown the fundamental advantages that can be gained through the use of a detailed and mechanistic modular model of the ramjet combustion process. The modular model developed in this work is however, limited to nonswirling sudden expansion flowfields. Similar approaches can be developed for swirl flow in subsonic combustors and for supersonic combustion applications. At the same time, fundamental model development work is required using unified Navier-Stokes approaches, and expanding the capabilities of these models to characterize flowfields with chemical reactions. This in turn indicates a need for the continued development of simple yet sufficiently general hydrocarbon chemical kinetics models as well as broadening the delineation of the regimes of model applicability.
- (d) <u>Ducted Rocket Model Development</u>: There is a dearth of information on the mixing characteristics of turbulent recirculating flows with embedded supersonic, underexpanded jets, yet this type of combined flowfield is central to the ducted rocket configuration. Clearly a need exists to explore the characteristics of these flows, both experimentally and through the development of theoretical models, in order to develop the understanding necessary to control them in practical applications.

2. RESEARCH STATUS

2.1 SPRAY FLAME MODEL

The spray flame model developed under this program applies to the near-dynamic equilibrium, thermal nonequilibrium limit of a two-phase flow. Thus, it is assumed that the mean velocity of both the droplets and the gas phase is nearly the same, but diffusion of particles relative to the gas phase is allowed. Gradient diffusion is assumed, with an apparent eddy viscosity that can be different from that which applies to the gas phase. The conditions required for the near-dynamic equilibrium assumption to be valid are clearly not met near the exit of a spray nozzle injecting fuel into a quiescent ambient. Nevertheless, the extent of the region in which this assumption is not valid is not well known, and it can be expected to become more valid as the spray flame flowfield develops. Thus it is of interest to investigate the capabilities of the approach, noting that when liquid fuels are injected using air streams to accomplish primary atomization, the near dynamic equilibrium assumption may indeed be reasonably valid over most of the flow.

2.1.1 Governing Equations

Governing equations for the two-phase spray flame flowfield are obtained following the development outlined in Ref. 1. A key element of this analysis involves the definition of the turbulent fluxes and their relationship to the gradients of the appropriate mean quantities. The "near" equilibrum concept simply recognizes that an exact equality in velocities between the phases does not exist, but that it is meaningful to characterize the global system with a single barycentric velocity in direct analogy with molecular diffusion. It is assumed that the droplets form a dilute suspension in the gas flow, and can be treated using continuum concepts. Thus the continuous distribution of droplet sizes within the spray flame is discretized into a number of classes, each of which contains all droplets in a given size range about the average range for the class. These classes are then treated as droplet-phase "species", and transport equations are written for each class. For example, if the droplet distribution function in terms of droplet radius is discretized into a number of radius intervals, the independent variable becomes the droplet number density for a given size, defined as the total droplet mass of a given size range per unit volume. The total droplet density is obtained by summing over the droplet size distribution function, and the partial and total particle densities are determined through solution of appropriate transport equations.

The diffusivities of the droplets will generally be different from that which pertains to the gas phase components, precluding a straightforward application of Fick's Law.to the global droplet-gas system. A multicomponent diffusion law can be developed, however, by treating each droplet class and the gas phase as a binary subsystem to which Fick's Law may be applied.

The basic governing equations are then as follows; where the nomenclature is as described in Table 3 following Eq. (17).

Global Continuity

$$\frac{\partial r \rho u}{\partial x} + \frac{\partial r \rho v}{\partial r} = 0 \tag{1}$$

Momentum

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \rho c_{vg} (\alpha_g + \sum_j \sigma_j \beta_{pj}) \frac{\partial u}{\partial r} \right] -$$
(2)

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Gas Phase Species Transport, ith Gas Phase Series

$$\rho u \frac{\partial \alpha_{i}}{\partial x} + \rho v \frac{\partial \alpha_{i}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \rho \frac{\varepsilon_{vg}}{Sc} \left[\frac{\partial \alpha_{i}}{\partial r} - \frac{\alpha_{i}}{\alpha_{g}} \left(\frac{1 - \Sigma \theta_{j} \beta_{pj}}{\alpha_{g}} \frac{\partial \alpha_{g}}{\partial r} + \Sigma \theta_{j} \frac{\partial \beta_{pj}}{\partial r} \right) \right] \right\} + \quad (3)$$

$$\dot{w}_{gi}^{C} + \dot{w}_{pij}^{F}$$

Droplet Phase "Species" Transport, jth Droplet Class

$$\rho u \frac{\partial \beta_{pj}}{\partial x} + \rho v \frac{\partial \beta_{pj}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \rho \frac{\varepsilon_{vg}}{Sc} \theta_{j} \left[\frac{\partial \beta_{pj}}{\partial r} - \frac{\beta_{pj}}{\beta r} - \frac{\beta_{pj}}{\beta r} \left(\frac{1 - \Sigma \frac{\theta_{k} \beta_{pk}}{\theta j}}{\alpha_{g}} \frac{\partial \alpha_{g}}{\partial r} + \Sigma \frac{\theta_{k}}{\theta_{j}} \frac{\partial \beta_{pk}}{\partial r} \right) \right] \right\}$$

$$+ \tilde{w}_{pj}^{F}$$
(4)

Mixture Energy Equation

 $\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ \left\{ r \rho \varepsilon_{vg} \left\{ \frac{1}{Pr} \frac{\partial H}{\partial r} + \left[h_g \frac{1}{Sc} \sum_{j} \theta_{j} \theta_{j} \beta_{pj} - \frac{h_g}{Pr} - \frac{1}{Pr} \left(\frac{Pr}{Sc} - 1 \right) h_g - \frac{1}{Sc} \sum_{j} \theta_{j} h_{pj} \beta_{pj} \right\} \right\} \\ \left(\frac{1 - \Sigma}{k} \frac{\theta_k}{\theta_j} \frac{\beta_{pk}}{\rho_k} \right) \frac{\partial \alpha_g}{\partial r} +$

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Mixture Energy Equation (cont'd),

$$\frac{1}{\Pr} \sum_{j} \beta_{pj} (\delta_{pj} - 1) \frac{\partial H_{pj}}{\partial r} + \frac{1}{\Pr} \left(\frac{\Pr}{Sc} - 1 \right).$$

$$\sum_{i} h_{ig} \frac{\partial \alpha_{i}}{\partial r} + \sum_{j} \left[\theta_{j} \frac{(h_{pj} - h_{g} \alpha_{g})}{Sc} - \frac{H_{pj}}{\Pr} \right].$$

$$\frac{\partial B_{pj}}{\partial r} + \left[B_{g} (1 - \frac{1}{\Pr}) - \sum_{i} \beta_{pj} \frac{\delta_{j}}{\Pr} \right] \frac{\partial (u^{2}/2)}{\partial r} - \frac{1}{Sc} \left(\sum_{j} \beta_{pj} h_{pj} \right) \left(\sum_{k} \theta_{k} \frac{\partial B_{pk}}{\partial r} \right) \right] = \rho u g - q'^{R}$$
(5)

Droplet Energy Equation for jth Droplet Class

$$B_{pj}\left(pu\frac{\partial h_{pj}}{\partial x} + pv\frac{\partial h_{pj}}{\partial r}\right) = \dot{q}_{pj} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\delta_{pj}}{Pr}p\varepsilon_{vg}\beta_{pj}\right)$$
$$-\frac{\partial h_{pj}}{\partial r} - \frac{\rho\varepsilon_{vg}}{Sc}\theta_{j}\left\{\frac{\partial B_{pj}}{\partial r}\right\} - \frac{\beta \beta_{pj}}{\rho r} - \beta_{pj}\left[\frac{\left(1 - \sum_{k=0}^{N}\beta_{pk}\beta_{pk}\right)}{\alpha_{g}}\frac{\partial \alpha_{g}}{\partial r}\right] + \frac{\beta \beta_{pj}}{\beta_{pj}}\left[\frac{\partial \beta_{pj}}{\partial r}\right] - \frac{\partial \beta_{pj}}{\partial r}\right] - \frac{\partial \beta_{pj}}{\partial r} - \frac{\beta \beta_{pj}}{\beta_{pj}}\left[\frac{\partial \beta_{pj}}{\partial r}\right] - \frac{\beta \beta_{pj}}{\beta_{pj}}\left[\frac{\partial \beta_{pj}}{\partial r}\right] - \frac{\partial \beta_{pj}}{\partial r} - \frac{\beta \beta_{pj}}{\beta_{pj}} - \frac{\beta \beta_{pj}}{\beta_{pj}}\right] - \frac{\partial \beta_{pj}}{\beta_{pj}} - \frac{\beta \beta_{pj}$$

The mixture density is given by the quation of state

$$\rho = P / [R_0 T_g(\sum_{i}^{\alpha} \frac{W_i}{W_i})]$$
 (7)

where W_i is the molecular weight of gas phase species i, Ro is the universal gas constant, and T_a is the local gas temperature.

To close the equation set and complete the model, a variety of additional submodels are required. These include models for the various production rate terms \dot{w}_{gi}^C , \dot{w}_{pj}^F , and \dot{w}_{pij}^F ; an expression for the thermal energy transferred to the droplets, \dot{q}_{pj} and the radiative energy transfer from the system, \dot{q}_i^R ; a droplet tracking scheme; and a turbulence model to define the effective gas-phase eddy diffusivity, ε_{vo} .

Turbulence Model

Turbulent transport, including the effects of buoyancy, is modeled using a two-equation formulation along with a temperature fluctuation equation. This results in a "three-equation" formulation, developed under a modified version of the Boussinesq hypothesis in which density fluctuations are neglected everywhere except when they appear in a buoyancy term. Writing density fluctuations in terms of temperature fluctuations leads to a formulation in which the buoyancy term in the turbulent kinetic energy balance is related to the root mean square of the temperature fluctuation, (Ref. 2) Thus the turbulence model is given by

$$\rho \varepsilon_{vg} = \mu_T = c_{\mu} \frac{k^2}{\epsilon}$$
 (8)

in which k and ε are obtained through solution of the equation for

Turbulent Kinetic Energy

$$\rho u \frac{\partial k}{\partial x} + \rho v \frac{\partial k}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial r} \right) + \nu_T \left(\frac{\partial u}{\partial r} \right) - \rho \varepsilon + \rho g \beta C_u \left(q k \right)^{\frac{1}{2}}$$
(9)

Turbulent Kinetic Energy Dissipation Rate

$$\rho u \frac{\partial \varepsilon}{\partial x} + \rho v \frac{\partial \varepsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{T}}{\sigma_{\varepsilon}} \frac{\partial \varepsilon}{\partial r} \right) + C_{1} \frac{\varepsilon}{k} \mu_{T} \left(\frac{\partial u}{\partial r} \right) - C_{2} \frac{\rho \varepsilon}{k} + C_{3} C_{u} \rho g \beta \varepsilon (q/k)^{\frac{1}{2}}$$
(10)

and the temperature fluctuation, $[(T')^2]^{1/2} \equiv q$ is obtained through the solution of a

Temperature Fluctuation Transport Equation

$$\rho u \frac{\partial q}{\partial x} + \rho v \frac{\partial q}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{T}}{\sigma_{g}} \frac{\partial q}{\partial r} \right) + C_{gl} \mu_{T} \left(\frac{\partial T}{\partial r} \right) - C_{gl} \rho \frac{\epsilon}{k} q \qquad (11)$$

This formulation introduces seven adjustable constants and three turbulent exchange coefficients. For most of the work described in this paper a single set of constants and coefficients was used in the turbulence model, as noted in Table 1. The basic turbulence model coefficients: Cµ, C_1 , C_2 , σ_k , and σ_ϵ were obtained from an extensive study of turbulent flowfield modeling reported in Ref. 3 while the coefficients used in the buoyancy modeling C_3 , C_4 , C_{ql} , C_{q2} , and σ_q were evaluated through comparison of nonreacting hot jet predictions with experimental data.

Table 1 Turbulence Model Constants

Parameter	Cµ	C 1	C ₂	C,	C 4	С ₉₁	c _{g2}	σ _k	σg	σ
Value	0.09	1.44	1.84	2.0	0.5	2.7	1.8	1.0	1.3	0.7

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Droplet Tracking Methodology

The spray flame model requires a droplet tracking and category readjustment methodology, since the rate processes result in droplet size changes and these, and the diffusion of droplets of different classes, alter the droplet distribution at each local point in the flow. At each step in the computation a new average size for each class must be defined, based on the alterations that result from diffusion and rate processes. This procedure follows the methodology outlined in Ref. 4; in it the appropriate drop-size average is defined through conservation of mass and conservation of the parameter defining the dominant rate process affecting droplet size. Thus, if the rate process is dependent on radius to the power q, the appropriate expression for the new average radius is given by

$$\overline{r}_{j}^{n+1,m} = \left\{ \frac{\beta_{pj}^{k} + \Delta\beta_{pj1} + \Delta\beta_{pj2} + \Delta\beta_{pj3}}{\frac{\beta_{pj}}{(r_{j}^{n,m})_{k}^{3-q}} + \frac{\Delta\beta_{pj1}}{(r_{j}^{n,m+1})^{3-q}} + \frac{\Delta\beta_{pj2}}{(r_{j}^{n,m})^{3-q}} + \frac{\Delta\beta_{pj3}}{(r_{j}^{n,m-1})^{3-q}} \right\}^{\frac{1}{3-q}}$$
(12)

where the averaging has been done assuming a three-point explicit finite difference scheme. The term $\beta_{pj}^{n,m}$ is the mass fraction of droplet class j at grid point n,m, the three diffusional components that contribute to the droplet class j at n+1, m are $\Delta\beta_{pj1}$, $\Delta\beta_{pj2}$ and $\Delta\beta_{pj3}$; β_{pj}^{k} is the contribution from finite rate processes. Knowing the mass fraction and size, the number density of droplets of class j at point n+1,m is then determined from

$$N_{j}^{n+1,m} = \rho^{n+1,m} \beta_{pj}^{n+1,m} / \left[\frac{4}{3} \pi \rho_{L} (r_{j}^{n+1,m})^{3}\right]$$
(13)

Note that the commonly used Sauter mean diameter (SMD), given by the expression $d_{eff}=\Sigma N_j d_j^3 / \Sigma N_j d_j^2$ implies a d_i^2 or surface area dependent rate process, i.e., q=2 in Eq. (12). However, the " d^2 " law for vapor-izing droplets implies a rate process that is proportional to the droplet diameter, so that, in Eq. (12) q=1. Somewhat different average radii will result depending on the governing rate process, and examination of calculational results shows that the use of q=2 (i.e., the SMD definition) in Eq. (12) yields a slightly different overall spray development than use of q=1 for a vaporizing spray. This difference is small for the conditions considered in this report, but in situations in which several different droplet-scale rate processes are occurring, the choice of average diameter definition may become more critical. Indeed under some circumstances it may be necessary to define more than one average diameter for each class of droplets.

Thermal Energy Transfer Terms

Two thermal energy transfer terms appear in the mixture energy and droplet-phase energy equations. These are \dot{q}^R , appearing in the mixture energy equation, which represents thermal energy transferred out of the flame by radiation, and \dot{q}_{pj} in the droplet energy equation, which represents a transfer of thermal energy to the droplets from the gas phase. Radiation from the flame to the surroundings is assumed to be dominated by gas phase CO₂ and H₂O emission, and is defined by an empirical expression, similar to that used in Ref. 5:

$$\dot{q}^{R} = 6.68 \times 10^{-12} T^{4} [\alpha_{H_{2}0} e^{e \times p(-1.49 \times 10^{-3}T)} + \alpha_{CO_{2}} e^{e \times p(-1.81 \times 10^{-3}T)}]$$
(14)

yielding \dot{q}^{R} in BTU/ft²-sec with T in ^{O}K .

yielding \dot{q}^R in BTU/ft²-sec with T in °K.

Energy transfer between gas phase and particle is accounted for through relationships obtained (Ref. 6) using the classical spherical droplet, flame sheet approach and solving the resulting governing equations for the droplet heat and mass transfer processes. For a vaporizing droplet, and accounting for droplet-gas heat transfer resulting from both conduction and radiation, this yields an expression for the energy transfer to the droplet of the form

$$\dot{q}_{pj} = \frac{3B_{pj}}{r_j \rho_L} \rho \left\{ \frac{\lambda N u}{2r_j} \left[\left(T_g - T_L \right) - \frac{L}{C_p} \right] - \epsilon \sigma \left(T_L^4 - T_g^4 \right) \right\}$$
(15)

Production Rate Terms

Three species production rate terms appear in the formulation. These involve production of gas phase species i through gas phase chemical reaction, \dot{w}_{gi}^{C} , production of droplet class j from other droplet classes through the effects of vaporization and combustion, \dot{w}_{pj}^{F} , and production of gas phase species i through vaporization or combustion of droplet class j, \dot{w}_{pj}^{F} .

The mass change of droplet class j per unit volume of mixture per unit time is evaluated using the classifical spherical droplet-flame sheet model. Thus the rate of change of droplet mass is given by

$$\hat{w}_{pj}^{F} = 3\beta_{pj} \frac{\lambda}{C_{p}\rho_{L}r_{j}^{2}} \ln (1+B)$$
(16)

where the transfer number, B, is given by

$$B = \frac{1}{\Gamma} \left[C_p(T_g - T_d) + \frac{QYO, \infty}{1} \right]$$
(17)

The species produced from the droplet class j will be either fuel, in the case of vaporization, or CO_2 and H_2O if the droplet is burning. In the model described in this report, the droplet is assumed to burn if suffi-

cient oxygen is present in its immediate environment; otherwise a pure vaporization process takes place. Thus if $\alpha_{0,2} \ge 0.001$, the present model produces CO_2 , H_2O (and excess fuel) from a complete combustion process in the flame sheet, and otherwise only gas phase fuel is produced. This lower limit is of course arbitrary.

Gas phase chemical kinetics are evaluated using the advanced quasiglobal formulation described in Ref. 7. This approach includes models for the fuel pyrolysis process that occurs in high temperature, oxygen deficient regions, and thus eliminates the inaccuracy evident in the original quasiglobal model formulation (Ref. 8) when applied to fuelrich combustion. In the advanced guasiglobal kinetics approach, the fuel to be modeled is broken down into aromatic and aliphatic components, modeled using rates developed for toluene and iso-octane, respectively. That is, the model fuel component which can be treated as aromatic is assigned rates which have been developed by extensive comparison of toluene predictions with experimental data, and the model fuel component that can be treated as aliphatic is assigned the rates developed for iso-octane. Each of these fuels break down into secondary fuels, C₂H₂ from toluene and C_2H_4 from iso-octane, following the pure pyrolysis pathway, as well as undergoing partial oxidation by attack from both 0_2 and OH. The secondary fuels then react with the remaining OH and 0_2 , and the wet CO mechanism follows.

For the computations to be described in this report, the fuel was pentane, so that only the aliphatic component needed to be included in the kinetics formulation. Since NO_x -formation reactions were also neglected, the gas-phase kinetics model used for these computations involved the 20 reactions among the 10 species shown in Table 2.

TABLE 2. ADVANCED QUASIGLOBAL KINETICS MODEL FOR ALIPHATIC FUELS

$FUEL = C_N H_M$

(a) SUBGLOBAL STEPS

 $k_{F} = AT^{B}exp(-E/RT)$

SUBGLOBAL MECHANISM	٨	. В	E/R	POWER DEPENDENCE
Primary Fuel				
$C_{NH_{M}} - \frac{N}{2}C_{2}H_{4} + (\frac{M-2N}{2})H_{2}$	1.0473 E12	0	3.5229 E3	[C5H12]1.0
$C_{N}H_{M} + \frac{N}{2}O_{2} - NCO + \frac{M}{2}H_{2}$	1.2900 E9	1	2.5160 E4	[C5H12] ^{0.5} [02] ^{1.0}
$C_{N}H_{M} + 0H - (\frac{2N-1}{4})C_{2}H_{4} + 0.5 CO + 0.5 H_{2}O + (\frac{M-2N+1}{2})H_{2}$	2.0000 E17	0	1.4919 E4	[с ₅ н ₁₂ [^{1.0} [он] ^{1.0}
Secondary Fuel				
$C_2H_4 + 6 \text{ OH} - 2 \text{ CO} + 2 H_2O + H_2$	2.2020 E15	o	1.2079 E4	[с ₂ н ₄] ^{1.0} [он] ^{1.0}
C2H4 + 2 OH 2 CO + 3 H2	2.1129 E27	-3.0	6.3062 E3	[с ₂ н ₄] ^{1.0} [он] ^{1.5}
$c_{2}H_{4} + M = c_{2}H_{2} + H_{2} + M$	2.0893 E17	: 0	3.9810 E4	[C ₂ H ₄] ^{1.0} [M] ^{1.0}
$C_2H_2 + 6 \text{ DH} - 4 H_20 + 2 CO$	4,7850 E15	0	1.3883 E4	[с ₂ н ₂] ^{1.0} [он] ^{1.0}
C ₂ H ₂ + 2 OH 2 CO + 2 H ₂	2.8000 E16	0	0	[C2H2] ^{1.0} [OH] ^{1.5}

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(b)	ELEMENTARY STEPS	
k _f	= AT ^B exp(-E/RT)	

ELEMENTARY MECHANISM	٨	8	E/R
со + он = н + со ₂	4.0000 E12	0	4.026 E3
он + н ₂ = н ₂ 0 + н	2.1900 E13	0	2.5900 E3
$0H + 0H = 0 + H_20$	6.0230 E12	o	5.5000 E2
0 + Н ₂ = Н + ОН	1.8000 E10	1.0	4.4800 E3
$H + 0_2 = 0 + 0H$	1.2200 E17	-0.91	8.3090 E3
0 ₂ + H ₂ = 0H + 0H	1.7000 E13	O	2.4070 E4
$(0 + 0_2 = 0 + 0_2)$	3.0000 E12	0	2.5000 E4
M + O + H = OH + M	1.0000 E16	0	0
M + H + H = H ₂ + M	5.0000 E15	0	0
- м + н + он = н ₂ о + м	8.4000 E21	-2.0	0
$M + CO + O = CO_2 + M$	6.0000 E13	0	0
$M + 0_2 = 0 + 0 + M$	2.5500 E18	-1.0	5.9380 E4

TABLE 3. NOMENCLATURE FOR EQ'S. 1-17

R transfer number, defined by Eq. 17 δ_{pj} ratio of droplet class j and gas phase thermal diffusivities = C_{ri} C_{rm} Cp C1 C2 liquid phase specific heat . ۲. آ C_{pg} τ_{ρj} Te_{vg} coefficients in turbulent kinetic energy dissi-[1] pation rate equation, defined in Table 1. turbulent kinetic energy dissipation rate 3 ε. ٤, ۲ (p³ droplet phase thermal diffusivity, class j coefficients in temperature fluctuation equa- C_q { tion, defined in Table 1. ε_{vg} gas phase eddy viscosity Cμ eddy viscosity coefficient, defined in Table 1 gas phase thermal conductivity λ turbulent effective viscosity = $\rho \epsilon_{vq}$ droplet emissivity e μ gravitational constant g Þ mixture density Mixture total enthalpy per unit mass of mixture н liquid density $= h_{g} + \Sigma \mathcal{E} h_{j} + u^{2}/2$ ρ_ι ambient density ρ__ hg Static enthalpy of gas phase per unit mass of Stefan-Boltzmann constant σ mixture = $\Sigma \alpha_1 h_1(T)$ ratio of eddy viscosity of droplet class j to °j gas phase eddy viscosity = Evj/Evg Static enthalpy of droplet class j per unit ^hрј mass of droplet class j effective "Prandtl number" for turbulent kineto, Ĵgi gas phase species i diffusional flux ic energy, Table 1 effective "Prandtl number" for temperature Ĵ_{pj} droplet phase species j diffusional flux ٥a fluctuation, Table 1 turbulent kinetic energy k effective "Prandtl number" for turbulent energy σG k_f forward reaction rate coefficient, Table 2 dissipation, Table 1. Ł latent heat of vaporization per unit mass Ň_j number density of dropiets of class j, Eq. 13 Nu Nusselt number for gas-droplet heat transfer ø pressure Pr turbulent Prandtl number q root-mean-square temperature fluctuation á' energy transfer from mixture by gas-phase radiation, Eq. 14 φ_{pj} energy transfer to droplet class j, Eq. 15 Q heat of vaporization radial coordinate r r j radius of droplet of class j Ro universal gas constant Sc turbulent Schmidt number Tg gas phase temperature Ţ gas phase temperature fluctuation TL. droplet temperature u axial velocity radial velocity ۷ .C "gi production of gas phase species i through chemical reaction production of droplet phase class j through ₩pj effects of vaporization, combustion, and adolomeration, per unit volume of mixture per unit time production of gas phase species i through vaporization or combustion of droplet class j. per unit volume of mixture ₩_i molecular weight of species i × axial coordinate Yo oxygen concentration, fraction of gas phase ٩ mixture mass fraction of gas phase = $\Sigma \alpha_i$ ۵, mixture mass fraction of species i ₿_{pi} mixture mass fraction of droplet class j

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2.1.2 Comparison with Experimental Results

Vaporizing Spray

In Ref. 9, Shearer, et al. describe detailed measurements of mean velocity, total concentration (both liquid and vapor phase), and Reynolds stress which were made in a two-phase Freon-ll/air jet mixing with still air. The jet was produced by the injection of Freon-11 into the air using an air-atomizing nozzle; the initial liquid-phase Freon mass fraction was 0.87. Shearer, et al. do not report droplet distributions; however, they give the initial SMD (Sauter mean diameter) of the Freon-11 droplets as 29 microns. The injection temperature of the Freon-11 was just below its saturation temperature, which in turn was just below the ambient air temperature. Thus the vaporization process for this jet was driven primarily by concentration gradients. Within the context of the model, this vaporization process was approximated by assuming a transfer number, β . of ten, in the droplet vaporization expression, Eq. (16). Vaporization was assumed to initiate when the droplet temperature reached the saturation temperature. An assumed initial droplet distribution, obtained from literature data for airatomizing nozzles, was used to initiate the calculations; this distribution, shown in Fig. 1, has a 29 µ SMD. All other initial conditions (i.e., velocity, temperature and droplet mass fraction, turbulence energy and dissipation rate) were taken to be uniform across the jet. All droplet classes were taken to diffuse at the same rate as the cas phase, i.e., θ_{i} =1 for all j. The phenomenon of phase separation, or relative diffusion, is included in the formulation but in the absence of detailed data θ_i must be established parametrically, so that $\theta_i = 1$ provides a reasonable baseline case.

Axial variations of centerline velocity and species mass fractions are compared with the data of Shearer, et al. in Fig. 2. As noted on the figure, these computations have been carried out for a turbulent Prandtl number of 0.70. These results indicate that the predicted velocity profile compares reasonably well with the experimental results,

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but that the centerline Freon concentration (both liquid and vapor phase) is somewhat underpredicted. More accurate predictions of the centerline Freon concentration can be achieved by using a unity turbulent Prandtl number assumption, but results obtained with this assumption strongly underpredict the width of the concentration profile. As can be seen from Fig. 3, the present computations (at a turbulent Prandtl number of 0.70) provide very accurate predictions of the shape and width of the concentration profiles.

Radial profiles of mean axial velocity are also predicted very well by the vaporizing spray jet model, as shown by the results presented in Fig. 4. Note that, despite its two-phase nature, the vaporizing spray jet exhibits the profile similarity behavior expected of an axisymmetric single-phase jet into still air.

The analytical model described here provides, in addition to the mean profile results already discussed, a variety of information with respect to the development of the spray. For example, the evolution of the drop size distribution in the spray is an output of the computation, and results for this parameter are shown in Fig. 5. The drop size distribution evolution is shown here for the centerline and an r/x value of 0.10, which corresponds roughly to the half-radius of the spray jet. Of interest is the fact that as the number of droplets decreases, the distribution remains roughly the same, so that the SMD, for example, shows little change. The nearly vertical lines on Fig. 5 represent the average diameter for each class at each value of X/D; the fact that they are nearly vertical indicates little change in mean diameter is occurring despite a nearly two-order-of-magnitude decrease in droplet number density. Thus the mean diameter of a spray distribution does not, from these results, appear to be a good indicator of the spray vaporization rate by itself.

Burning Spray

Mao, et al. (Ref. 10) report results for a spray diffusion flame. The experimental apparatus and measurement techniques used are quite similar to those used in the vaporizing spray study of Shearer, et al. already dis-

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Figure 3. Radial Variation of Freon Concentration Vaporizing Spray Jet. Data from Ref. 9 Model Predictions at X/D = 235



Figure 4. Radial Variation of Axial Velocity, Vaporizing Spray Jet. Data from Ref. 9





cussed. For the spray flame experiments, Mao et al. utilized n-pentane as a fuel, with an initial droplet distribution having a SMD of $35 \,\mu$ m. Measurements include centerline velocity, fuel species, and temperature distributions, as well as radial profiles of velocity and temperature. Analysis of these data using the locally-homogeneous-flow (LHF) approximation is also reported in Ref. 10.

The calculations carried out using the spray flame model described in this report were initiated using a droplet distribution similar to that used for the nonburning spray, but adjusted to yield an SMD of 35 µm. Initiation of the flame in the calculations is provided by the droplet flame sheet assumption: since an air-atomizing nozzle was used sufficient oxygen is available at the injector exit to initiate chemical reaction. This is an artifice, but it does provide an appropriate flame initiation zone to begin the computations. This initial reaction quickly exhausts the available oxygen, so that the bulk of the droplets vaporize in a hot fuel rich region in the interior of the flame. The fact that in the computations the bulk of the droplets do not enter directly into the combustion process is fully supported by experimental observations made by Mao et al. Gas phase combustion is described in the model using the advanced guasiglobal approach described in the preceding section, and gas phase thermal radiation is also included. This latter phenomenon was found to strongly affect the development of the flame, as described below.

A comparison of predicted centerline temperature with the temperature experimentally measured in the pentane spray flame is shown in Fig. 6. The overall profile shape is very well predicted, particularly for X/D>200, but the predicted temperature is everywhere higher than that measured. Here radiation may play a role, both in the model and in the experiment. For X/D<200, the predicted temperature is substantially in excess of that measured. In these calculations, the droplets vaporized by X/D=100, whereas experimental observations of droplets to 150 diameters were reported. This suggests that the computed droplet vaporization rate is too high, and that the flame sheet model for droplet consumption on the edge of the flame is an oversimplification. Nevertheless, noting that there is no normalization in this comparison (other than division of the axial distance by the physical jet diameter), these results are very encouraging.

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Both thermal radiation and buoyancy effects had to be included in the computational model in order to achieve a reasonable representation of the spray flame development. A number of parametric computations were carried out during the development of the approach, the results of which illustrate the effects of the neglect of these important phenomena. For example, the results shown in Fig. 7 indicate centerline temperature distributions obtained without including the effects of buoyancy, but with and without incorporation of the effects of gas-phase thermal radiation. The measured centerline temperature peaks at a value of some 1800°K. Without incorporating the effects of gas-phase thermal radiation, the predicted centerline temperature continues to increase, eventually reaching the adiadatic flame temperature for stoichiometric pentene-air combustion. Incorporating radiation losses, the model prediction of centerline temperature is much reduced with, in this case, a predicted temperature peak of only 1550°K.

Buoyancy influences both the mean flow and turbulence structure in the spray flame, and the relative effects of buoyancy increase as the magnitude of the buoyancy-induced body force term in the momentum equation increases relative to the momentum flow per unit area term. Since in a jet-into-stillair the local momentum flow per unit area is continuously decreasing with axial distance, at the same time as the temperature and therefore body force term increases, buoyancy effects can be expected to always exert some influence on the development of a spray flame in a quiescent ambient. The magnitude of this influence is illustrated by the results shown as Fig. 8, which presents computed centerline temperatures obtained including the effects of gas-phase thermal radiation, but with and without incorporation of the effects of buoyancy as the mean flow. Note that these results do not include the influence of buoyancy effects on the turbulent mixing rate. The results shown in Fig. 8 show that there are very large effects of buoyancy in this spray flame structure, since with mean-flow buoyancy effects included the calculation represents the shape of the centerline temperature profile quite well, particularly with respect to the rapid decay of centerline temperature downstream of the location of the temperature. However, the effects of incorporation of mean flow buoyancy without incorporating the corresponding buoyancy-turbulence structure effects produce a quite

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Figure 7. Centerline Temperature Distribution Reacting n-Pentane Spray Jet, With and Without Gas-Phase Thermal Radiation. Effects of buoyancy neglected. Data from Ref. 10.

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different result when computed centerline velocity is compared with experimental data. This is demonstrated by the results shown in Fig. 9 where it can be seen that with mean-flow buoyancy, an increase in centerline velocity is observed for 100 < X/D < 300. Clearly the data do not support this result. However, if the effects of buoyancy on the turbulent mixing process are included, through the buoyancy terms appearing in Equations (9) and (10), this centerline velocity increase phenomenon is to a large extent avoided. This result is shown by the centerline velocity variation results shown in Fig. 10, which correspond to the centerline temperature results of Fig. 6. These results show that the effects of buoyancy become apparent at around X/D=200, and result in a reduced rate of centerline velocity decay compared to the experimental data. The underprediction of the velocity decay rate is consistent with the overprediction of the centerline temperature, one effect of which would be to increase the magnitude of the buoyancy effect. Yet velocity profiles, Fig. 11, agree extremely well with the data for X/D>200; these profiles, while normalized with the centerline velocity (as was the data) are not normalized with respect to the physical coordinate in a way that would mask disagreement. Indeed, the normalization used indicates that the computations correctly model the spread rate of the spray diffusion flame, at least for X/D>170.

The accuracy of the spread rate prediction is also indirectly supported by comparison of the calculated and measured Reynolds stress component. This result, shown in Fig. 12, shows a very good level of agreement both in magnitude and location of the maximum shear stress. It has been established for single phase jets into quiescent ambients that the rate of spread of the jet is controlled by the peak shear stress levels encountered in the profile. so that the good level of agreement seen in Fig. 12 supports the velocity profile agreement displayed in Fig. 11.

Finally, computed and measured temperature profiles are compared in Fig. 13. Here it is evident that in the center of the flame the model predicts higher temperatures than are experimentally observed. Again, both droplet vaporization rate and gas phase radiation submodels are implicated in this disagreement. Other factors may enter as well. For example,

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Figure 11. Radial Velocity Profile Comparison, n-Pentane Spray Flame. Calculation includes gas-phase thermal radiation, meanflow and turbulence structure buoyancy effects. Data from Ref. 10

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Figure 13. Comparison of Computed and Measured Temperature Profiles, Pentane Spray Flame

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although the flow has been treated as fully turbulent, in both the original experiment documentation and in this work, it may have actually involved a laminar or transitional flow in the first 100 diameters or so. If this were the case, a slower rate of mixing than predicted herein would have existed, resulting in lower centerline temperature than predicted by this fully turbulent model.

2.1.3 Discussion

In assessing the performance of the spray flame model just described, it is important to keep in mind the important effects of the the strong coupling inherent in a spray diffusion flame. For the particular flow-field considered this coupling includes not only the mixing and kinetics, but also the effects of phase change, radiation, and buoyancy. Taking just one of these as an example, the effects of inclusion of thermal radiation were found to be significant in these calculations, accounting for centerline temperature differences ranging from 400°K to 1000°K. This level of temperature difference is significant with respect both to chemical kinetic and buoyancy effects. The buoyancy model is also worth noting, since results of additional computations clearly showed that neglecting the influence of buoyancy on the turbulent structure produced erroneous results. Thus, while attention in assessing the performance of this model may be focused on the use of the near dynamic equilibrium hypothesis, it is not altogether clear that this hypothesis exerts a dominant effect on the overall results.

Overall, the approach described in this paper provides a reasonably valid picture of the development of a spray diffusion flame. Moreover, it provides a computational tool which can usefully be applied to the parametric examination of the many physical and chemical interactions that underlie spray flame phenomena, both from a purely theoretical standpoint and in conjunction with detailed spray flame measurements. The approach also provides the basis for further development, for example through relaxation of

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the limitation to near dynamic equilibrium in the spray transport process. Clearly, the model is complex, and involves a great variety of phenomena. But spray diffusion flames are themselves complex, and careful theoretical and experimental study is required to determine where model simplification may justifiably be made.

From a computational standpoint the complexity of the model is actually more apparent than real. Even with detailed finite-rate chemistry as described by the guasiglobal kinetics model, computation of the n-pentane spray flame considered here, carried out to an axial distance of 500 nozzle diameters, requires only about 30 minutes of CPU time on a CDC 7600. Computational times on more advanced computers can be expected to be considerably less. What the model provides for the investment in computer time is substantial detail with respect to the general structure of the spray flame flow field. For example, detailed temperature contours in the spray flame can be presented to illustrate the structure of the flame, as in Fig. 14. When compared with droplet distributions, as shown in terms of total mass fraction in liquid form on Fig. 15, conclusions can be drawn as to the mechanisms which the modeling indicates will dominate in the flame structure. Comparison of Figs. 14 and 15 shows that the bulk of the droplets are found in regions on the flame in which local temperature is greater than 800°K, but below 1200°K. Comparison with gas-phase oxygen profiles shows that this is a very fuel-rich region. Thus, except for an initial short region near the nozzle exit where temperatures range from 1600°K to 2000°K (and which is an artifice of the assumption that droplets burn, rather than vaporize, if $\alpha_0 > 0.001$), vaporization is the primary mechanism responsible for the reduction in liquid-phase mass fraction. Combustion occurs only in a narrow region surrounding the droplet cloud, and for X/D<80. is a low-temperature, fuel-rich process involving the mechanisms of pure and oxidative pyrolysis. Beyond X/D~80, the liquid-phase mass fraction drops below 0.05 and there is a sudden and rapid increase in the reaction rate as indicated by the widening of the predicted flame shape seen on Fig. 14. This behavior is qualitatively in agreement with that observed experimentally, although these predictions indicate its occurrence rather sooner in the spray flame development than was otherwise observed.

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It should also be noted that the particular experimental configuration selected for study in this work was not ideal from the standpoint of modeling complexity. In particular, the quiescent ambient introduces larger effects of buoyancy than would be the case in a coflowing situation. Indeed, it is possible to design an experiment which satisfies the assumptions of the analysis much more closely than that considered here, for example, with respect to the near-dynamic equilibrium assumption, while at the same time reducing the magnitude of the buoyancy effects. By doing this, and carefully comparing the experimental results with analytical predications it would be possible to considerably enhance the characteristics of the multiphase spray flame model described in this work. By inference, then, questions of droplet-scale modeling, droplet-droplet and turbulence interaction could all be addressed in a step-by-step manner.

Finally, the results presented here are, in terms of level of agreement with the data, substantially similar to those reported in Ref. 10. The results described in Ref. 10 were obtained using a model which ignores two-phase flow effects, finite-rate vaporization, finite-rate gas phase kinetics, gas-phase thermal radiation, and buoyancy phenomena. Instead, the model utilized in Ref. 10 incorporates a turbulence-chemistry interaction model based on an assumed probability distribution function approach. Two-phase flow, finite-rate vaporization, finite-rate gas phase kinetics, gas-phase thermal radiation, and buoyancy are all physically real phenomena, and the parametric investigation reported above indicate the magnitude of their effects. Thus, the agreement with experiment of a theoretical treatment that ignores each of these phenomena in succession requires further explanation.

2.2 MODELING OF BORON COMBUSTION PROCESSES

Boron slurry fuel combustion is a complex phenomenon involving two-phase flow and finite-rate reaction processes in the gas phase and in the particle surface. In a slurry fuel, the boron is generally in the form of micron-sized particles suspended in a carrier hydrocarbon. As the hydrocarbon carrier burns, the boron is heated to the ignition temperature, and

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it then subsequently burns with exposure to sufficient oxygen. One of the difficulties encountered in boron combustion is that a surface oxide layer can form on the particle. This oxide has a boiling point below that of the metal, so that the boron combustion process involves a diffusion of oxidizing gases through the liquid oxide layer with a surface reaction taking place at the particle/liquid interface. Since this is a slow process, one strateqy for obtaining high boron combustion efficiencies is to limit the amount of oxygen reaching the surface of the particle during the heat-up process; i.e., carrying out the particle heatup in a regime which is fuel-rich relative to the hydrocarbon carrier, and then exposing the hot particles and remaining fuel to additional air. This form of staged combustion is difficult to achieve in practice, and the development of boron slurry fueled combustors could be materially aided by the availability of analytical design tools. The modular model described in the next section of this report provides the framework for the type of design tool that could be used for this purpose, but its extension to the analysis of boron slurry combustion requires the development of submodels of the boron combustion process. These submodels are the principal focus of the work carried out under this portion of the AFOSR-sponsored research at SAI.

2.2.1 Boron Combustion Models

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Single-particle boron ignition and combustion models have been reported by King (Refs. 11, 12), Meese and Skifstad (Ref. 13), Vovchuck et al. (Ref. 14), Mohan and Williams (Ref. 15) and Edelman, et al. (Refs. 16, 17). The component equations that make up each of these models are summarized in Table 3, which also includes a review of the assumptions built into each of the models. The nomenclature for Table 3 is given in Table 4. In general, these formulations are based on the assumption of a spherical particle (except for the work of Mohan and Williams) and on the conservation equations for mass and energy. The momentum equation is not explicitly coupled into the equation set, but in certain of the models the relative velocity effect is accounted for through a Nusselt number correction on heat

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TABLE 4. SUMMARY OF AVAILABLE BORON IGNITION AND COMBUSTION MODELS

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	$ \left(\frac{4}{3} * r_F^* p_B c_{FB(S \text{ or } L)} * 4 * r_F^* X p_{B_2 0_3} c_{PB_2 0_3}\right) \frac{dT_P}{dE} * P_B (0_{RX}) - P_E (AH_{VAP}) - P_H AH_H * 4 * (r_P * X) $ $ \left[h (T T_P) * \sigma c \alpha_R (T_{RAD}^* - T_P^*)\right] $	s King
COMPLETE MEAT TEANSFER LQUATIONS	$(m_B c_{PB} + m_{B_2 0_3} c_{PB_2 0_3}) \frac{dT_p}{dt} = R Q - R_E M_{VAP} + 4 \pi r_2^* \cdot [h (T_g - T_p) + o o c (T_{PAD}^* - T_p^*)]$	Heese
	$-4 \pi \lambda r' \frac{d7}{dr} - 1_{0_2} H_{0_2}(1) + 1_B H_B(1_k) - 1_{B_2} H_{0_2}(1) - q_R^K$	Forchut
	$h c_{C} c_{C} \frac{dT_{C}}{dt} = q_{B} c_{B} R_{B} - q_{C} c_{C} R_{C} - L$	Matan
	$\frac{dT_{p}}{dt} = \frac{3}{2} \frac{a \lambda (H_{U})}{c_{s} c_{ps} R^{4} c_{p}} + \left\{ \frac{c_{p} (T_{q} - T_{p})}{e^{a} - 2} - L + A k_{s} \left[\frac{2 c_{p} p_{s} R}{a \lambda (H_{U}) y_{O_{2,s}}} \right] + \frac{M_{B}}{M_{O_{2}}} \Delta H_{R} - \frac{2 \sigma c R c_{p}}{a \lambda (H_{U})} (T_{p}^{*} - T_{w}^{*}) \right\}$	Edelsan
	$\left(\frac{4}{3} \pi r_{P}^{3} \rho_{B} c_{PBS} + 4 \pi r_{P}^{2} X \rho_{E_{2}O_{3}L} c_{PB_{2}O_{3}}\right) \frac{\sigma T_{P}}{\sigma \theta} = 4 \pi (r_{P} + X)^{2} (T_{P} - T_{P}) h$ EFLOW PHASE CHANGE OF EDRON, $T_{P} < 2450$	King
FEAT TRANSFER: CONDUCTION-CONVECTION	$(\frac{4}{3} + r_p^3 \rho_B \Delta H_m) \frac{df}{d\theta} = 4 + (r_p + \lambda)^3 (T_p - T_p) h$ AT Fritse CHILNGE, Tp = 2450, 0 < f < 1	
	$ (\frac{4}{3} * r_F^1 + r_6 + r_P^2 + 4 * r_P^2 + r_P^2 $	
Components	$(m_{\rm B} c_{\rm PB} + m_{\rm 20_3} c_{\rm PB_20_3}) \frac{dT_{\rm p}}{dt} + 4 + r_2^2 h (T_{\rm g} - T_{\rm p})$	Keese
	$h \rho_{C} c_{C} \frac{dT_{C}}{dt} \cdot (T_{C} - T_{D}) \frac{2\lambda}{D}$	Hoten
	$\frac{4}{3} * k^{3} e_{s} c_{ps} \frac{dT_{p}}{dt} = 4 * R^{3} h (T_{g} = T_{p}) \frac{a}{e^{a} - 1}$	Felson
	$ (\frac{4}{3} * r_p^2 r_g c_{PBS} + 4 * r_p^2 X p_{e_2 0_3 t} c_{Fe_2 0_3}) \frac{dT_p}{d\theta} + 4 * (r_p + X)^2 \sigma c \alpha_R (T_{RAD}^* - T_p^*) $	
HEAT TRANSFER: RATIATION	$(\frac{4}{3} + r_P^2 + E_E L^{H_E}) \frac{df}{d\theta} + 4 + (r_P + \chi)^2 \sigma \epsilon \alpha_R (T_{RAD}^* - T_P^*)$	King
	$ (\frac{4}{3} + r_F^3 p_E c_{FBL} + 4 + r_P^3 x p_{P_2 0_3 L} c_{FP_2 0_3}) \frac{dT_P}{d\theta} = 4 + (r_P + x)^3 \sigma c \sigma_{\overline{x}} (T_{EAD}^* - T_P^*) $	Moten Edelsan King
	$ \begin{pmatrix} \sigma_{P} \\ \sigma_{E} \\ c_{FB} \\ + \\ \sigma_{F_{2}} \\ \sigma_{3} \\ c_{FF_{2}} \\ \sigma_{3} \end{pmatrix} = 4 \\ s \\ r_{2}^{2} \\ \sigma \\ \alpha \\ c \\ (T_{F,D}^{*} - T_{P}^{*}) $	Murese
	$-4 \pm \lambda r^2 \frac{dT}{dr} = -4 \pm r_k^2 c \sigma \left(T_k^* - T_k^*\right)$	

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HEAT TRANSFER:		$-1.36 \ \epsilon \left(\frac{T_{c}}{1000}\right)^{4}$	th tien
RADIATION	⁴ π R' c _{ps} ^δ d t	- 4 x R ² O L (T ^x - T ^x)	[dilron
	$B_{(5,L)} + \frac{3}{4}D_{Z(g)} + \frac{1}{2}B_{2}D_{3(g)}$	TAST REACTION DIFFUSION LIMITED HAPPENS AT DXIDE-BORDH INTERIACE	Fing
	$B_{(S,1)} + \frac{3}{4} O_{2(g)} - \frac{1}{2} B_{2}O_{3}$	3(g) WORK BASED ON KING*S	Pirese
GAIDE LORMATION	$2BO_{2(g)} = B_{2}O_{3(g)} + \frac{1}{2}O_{2(g)}$ $B_{2}O_{3(g)} = 2BO_{(g)} + \frac{1}{2}O_{2(g)}$ $B_{2}O_{2(g)} = 2BO_{(g)}$	THERMAL EQUILIERIUM DIFFUSION CONTROLLED LOWER DXIDES ONLY AT SURFACE	Yovehuk
	$B_{(5)} + \frac{3}{4}O_{2(g)} + \frac{1}{2}B_{2}O_{3(L)}$	DIFFUSION CONTROLLED EQUILIBRIUM VAPORIZATION OF E.O. AND ABSORPTION OF O. IN THE LIQUID E.O. AT LIQUID- GAS SURFACE.	Poten
	$B_{(1)} + \frac{1}{2} O_{2(g)} - BO_{(g)}$ $B_{(1)} + \frac{3}{4} O_{2(g)} + \frac{1}{2} B_{2}O_{3(g)}$	FINITE-RATE KINETICS CONTROLLED	[de]ran
DAIDE CONSUMPTION	$H_2^0(g) + E_2^0(1) + 2HB0_2(g)$	DIFFUSION LIMITED ENDOTHERMIC REACTION RATE CONTROLLED EVAPORATION	King
	$H_2^{0}(g) \stackrel{f}{=} E_2^{0}(1) \stackrel{f}{=} 2HBO_2(g)$) WUPK BASED ON KING'S	Hrese
DIFFUSION THECHON GAS FILM	DIFFUSIVITY OF P203, HB02, H20 GAS THROUGH DJ.H2 • 4.3 • 10, P (VJ' RH 0H20.M2 Z = (rp + X) • 2 (rp + X H 0HB Z = (rp + X) • 4 (rp MCLAR FEMOVAL RATI	$H_{2} FILM ; J = ONE OF: P_{2}O_{3}, HEO_{2}, H_{2}O$ $\frac{P^{3}}{+ Y_{M_{2}}^{*}} = \sqrt{\frac{1}{(H_{N})_{3}} + \frac{1}{(H_{N})_{R_{2}}}}$ $\frac{P_{M}}{P_{1}R_{T_{p}}} (P_{H_{2}O, -} - P_{H_{2}O, SURF})$ $\frac{P_{1}O_{2}, N_{2}}{P_{1} + X_{1}R_{T_{p}}} (P_{HEO_{2}, SURF})$ $E OF GXIDE BY WATER$	King
ATES AND CONSTANTS	WORK EASED	OY KING'S	He ese
	$I_{O_2} = -6 = r^2 \frac{D}{RT} \frac{dP_{O_2}}{dr}$ ETC. B_2O_2 ,	$I_{BO} = -4 \pi r^2 \frac{D}{kT} \frac{dP_{BO}}{dr}$ P_2O_3, BO_2	Vevela
-	$R_{c} = 2 X_{a} D_{b} \rho_{a} / \rho_{c} d 0;$ $R_{B} = R_{c} = (q_{c} \rho_{c} R_{c} + t) / q_{b}$	UTWARD GAS-FRASE DIFFUSION OF B ₂ 0 ₃ P _b AT LOW TEMP. STAGE	Holen
	+16[7](A)) Y	CONTROLLED	1612-1

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	$H_{2}O(g)$, $HBO_{2}(g)$, $O_{2}(g)$, $B_{2}O_{3}(L,g)$, $B(x,L)$, $H_{2}(g)$	ting
	$H_{\tilde{z}}^{0}(g), H_{B0}^{0}(g), O_{2}(g), B_{\tilde{z}}^{0}(t,g), B_{(s,t)}, M_{2}(g)$	
AT THE SURFACE	$B_{(s,1)}, B_{(g)}, B_{(g)}, B_{2}O_{2}(g), E_{2}O_{3}(g), O_{2}(g)$	Vovrhu
	$B_{(s)}, B_2O_{2(g)}, O_{2(g)}, B_2O_{3(1,g)}$	Holar
	$B_{(s,L)}, B_2^{0}_{2(g)}, D_{2(g)}, B_{2(g)}$	Edelra
	HBO ₂ , P ₂ O ₃ , O ₂ , H ₂ O, M ₂	King
SFECTES FOUND	HB02, E203, 02, H20, N2	Herese
DEF SURFACE	B ₂ 0 ₃ , P ₂ 0 ₂ , 0 ₂	Vovchul
(GASE S)	$B_2 D_3, M_2, D_2$	Hotian
	е ₂ 0 ₃ , 0 ₂ , N ₂ , во	Edelrør
	SET EQUAL, TO 2.0	King
NUSSELT NUMBER	$(1 + 0.296 \text{ Fr}^{3/3} \text{ Re}^{3/3}) \sim \text{Nu}$ BASED ON RADIUS	Prese
	$Hu = 2 + 0.276 Fr \sqrt{3} Fe^{\sqrt{3}}$ $Pr = \frac{c_p v_q}{\lambda} Fe = \frac{2 F p_q (v_q - v_p)}{v_q}$	Edelran
	FOIL-OFF TIME OF OXIDE LAYER	
FUMMING TIME S	$t_{B} = \frac{r_{B_{2}O_{3}}(r_{2}^{*} - r_{1}^{*}) \Delta H_{YAP}}{3r_{2}^{*}(F/A)Q + h(T_{g} - T_{p}) + \alpha \sigma c(T_{FAD}^{*} - T_{p}^{*}) M_{P_{2}O_{3}}}$	Meese
	$T_{c} = \frac{\Gamma_{B} d_{k0}^{3}}{16 \mu_{E} \frac{\tilde{D}}{RT} P_{02}} = \frac{V_{F} - V_{F} - V_{E} d_{d0}^{3}}{V_{B} V_{B} V_{D} \frac{P}{R} \frac{\tilde{D}}{T} - \frac{1}{V_{E_{2}0_{3}}} \left[\ln \left[P - (1 - V_{E_{2}0_{3}}/V_{0_{2}}) P_{0_{2}} - \right] \right]$ L= OPLET (1= SUSIDON TIME	Yovchuk
	$t_{B} = \frac{c_{F} p_{f}}{B\lambda} - \left\{ \ln \left[1 + \frac{Q_{F} + c_{F}}{L} \left(T_{-} - T_{f} \right) \right] \right\}^{-1}$	
	$\frac{dr_{p}}{d\theta} = \frac{-R_{B}}{4 \pi r_{p}^{2} P_{B}} \qquad \frac{dx}{d\theta} = \frac{(R_{B}/2 - R_{E} - F_{H})(M^{2})P_{2}O_{3}}{4 \pi r_{p}^{2} P_{E_{2}}O_{3}}$	King
AND/OR	$\frac{dr_{B}}{dt} = -R \pi_{B} \pi_{B} = \frac{4}{3} \tau r_{1}^{3} r_{B} \qquad \frac{dr_{E_{2}} 0_{3}}{dt} = (R/2 - P_{E}) \pi_{E_{2}} 0_{3} \qquad \frac{4}{5} \tau (r_{2}^{3} - r_{1}^{3}) r_{E_{2}} 0_{3}$	Perse
CXIDE CHANGE	$dh = R_B = \frac{P_C}{C} = F_B = X k D / n = \frac{P_C}{C} = 2 \frac{X_A}{A} \frac{D_A}{C} \frac{F_A}{C} \frac{P_C}{C} d$	Motion
	$\frac{G(R^2)}{dt} = -a \lambda (Ku)$	[delean
, i	s p	1

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TABLE 5. NOMENCLATURE FOR EXPRESSIONS SUMMARIZED IN TABLE 3

5.1 KING'S MODEL liquid boron heat capacity (cal/gm°K) C_{PB1} solid boron heat capacity (cal/gm°K) CPBS liquid boron oxide heat capacity (cal/gm°K) C_{PB2}02 fraction of boron in the liquid phase gas-particle heat transfer coefficient (cal/cm²sec[°]K) h mass transfer coefficient for transport of boric oxide gas from k particle to free-stream (gm-mol/cm²atm sec) (MW)_R boron atomic weight (gm/gm-mol) (MW)B202 boric oxide molecular weight (gm/gm-mol) Nusselt Number Nu Ρ total pressure (atm) oxygen partial pressure in free stream (atm) P02 PB203, surf boric oxide partial pressure adjacent to particle surface (atm) ^P[°]₈₂03 boric oxide vapor pressure (atm) water gas partial pressure adjacent to particle surface (atm) P_{H2}0, surf HBO_ppartial pressure adjacent to particle surface (atm) PHB02, surf boric oxide partial pressure in free-stream (atm) P₈₂03, ∞ heat release of B(s) + $\frac{3}{4}O_2$ + $\frac{1}{2}B_2O_3(1)$ (cal/gm-mol) Q_{RX} heat release of B(1) + $\frac{3}{4}O_2 \rightarrow \frac{1}{2}B_2O_3(1)$ (cal/gm-mol) Q_{RX2} gas law constant, 82.06 atm-cm³/gm-mol°K R molar rate of boron consumption (gm-mol/sec) R_B R_E molar evaporation rate of boric oxide (gm-mol/sec) R_H molar rate of removal of B_2O_3 by water reaction (gm-mol/sec) boron particle radius (cm) rp T_ free stream gas temperature (°K) T_{CL} particle center temperature (°K) Tp particle temperature (°K) TRAD surroundings radiation temperature (°K) particle surface temperature (°K) Τs Vj X molecular volume of species j (cm³) oxide layer thickness (cm) D₈₂03.N2 diffusivity of gaseous boric oxide in nitrogen (cm²/sec) diffusivity of HBO₂ in mitrogen (cm²/sec) D_{HB02},N2 diffusivity of water gas in mitrogen (cm²/sec) D_{H2}0,N2 ۵н_н heat absorbed by reaction of H_20 with $B_20_3(1)(cal/gm-mol)$ ۵Hm heat of fusion of boron (cal/gm) ^{∆H}vap heat of vaporization of $E_2O_3(1)(cal/gm-mol)$

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۵	evaporation coefficient of boric oxide liquid
ap	surroundings absorptivity
α _t	thermal diffusivity of boron (cm ² /sec)
٥	Stefan-Boltzmann constant, 1.354-10 ¹² cal/cm ² sec°K ⁴
C	particle emissivity
v	Hertz-Knudsen impingement factor (gm-mol/cm ² atm sec)
θ	time (sec)
۹ ₈	buron density (gm/cm ³)
ρ _{Β20} 3	boric oxide density (gm/cm ³)
5.2 MODE	. OF MEESE AND SKIFSTAD
A	surface area, cm ²
с _р	specific heat, cal/g-°K
ď	particle diameter, cm
ε	activation energy for evaporation
۵H	heat of fusion of boron, cal/g
^{ДН} уар	heat of vaporization of boron oxide, cal/mole
h	convective heat-transfer coefficient, cal/cm ² -sec-°K
k	thermal conductivity, cal/cm-sec-°K
м	molecular weight, g/g-mole
m	mass, g
Р	pressure, atm
Pr	Prandtl number of the gas
Q	heat of combustion of boron with diatomic oxygen to form liquid
	B ₂ 0 ₃ , cal/mole; total energy, cal
R	molar rate of consumption of boron, g-mole/sec; gas constant
Rc	molar rate of evaporation of boron oxide, gm-mole/sec
Re	Reynolds number based on particle diameter and relative velocity
	between the gas and particle
r	radius, cm
۵r	oxide film thickness, r ₂ -r ₁ , cm
T	temperature, °K
t	time, sec
^х н ₂ 0	mole fraction of H_2^0 present in the gas
a	surrounding absorptivity (=1.0)
E	particle emissivity (=0.8)
λ	particle burning rate, cm/sec
ρ	density, g/cm
σ	Stefan-Boltzmann constant, cal/cm ² sec°K ⁴



TABLE 5. (Continued)

5.3 MOHAN	'S MODEL
С	average molecular velocity normal to the surface (cm/sec)
с,	heat capacity of B ₂ O ₃ (L)(cal/gm [°] K)
ב	diffusion coefficient (cm ² /sec)
d	diameter of particle (cm)
h	thickness (cm)
k	effective distribution coefficient related to the ratio of the
	mole fraction of O_{n} absorbed in $B_{n}O_{n}(k)$ to gas phase mole frac
k'	distribution ratio (liquid phase to gas phase 0, concentration
ι	sum of heat losses by radiation and conduction $\frac{2}{cal}$
Ρ	total ambient pressure (atm)
۹ ₈	heat liberated per unit mass of boron consumed at B (cal/g)
۵ ۹ ₀	heat absorbed per unit mass of B_2O_2 vaporized at C (cal/g)
Record	regression rate of the surface (cm/sec)
R°	universal gas constant (8.316•10 ⁻⁷ erg/gm-mole °K)
T	temperature (°K)
t	time (sec)
W;	atomic weight
x	mole fraction of O ₂ in the ambient atmosphere
Xa	ratio equilibrium vapor pressure of B_2O_3 at Tc to total pressur
۵	evaporation coefficient
£	emissivity
λ	gas phase thermal conductivity (cal/cm+sec °K)
P _B .C	density boron and B ₂ O ₂ (gm/cm ³)
т	time for the new combustion regime to appear (sec)
B,C	surfaces
5.4 VOVCHU	JK'S MODEL
C _P	molar specific heat
D	diffusion coefficient
ddo	initial diameter of the boron droplet
н _і	total enthalpy of species i
۵H _i	heat of reaction of species i
1 ₁	molar flux of species i
м _в	mass flow of the boron reacting in unit time
P	total pressure
P i	partial pressure of species i
Q _R K	radiative heat flux
R	universal gas constant
r	radius
T	temperature



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TABLE 5. (continued)

λ	thermal conductivity of gas
ν _i	molecular weight
vi	stoichiometric coefficients
Pi	density
0	Stefan's constant
۲r	droplet combustion time
Subscripts	_
в	(molten) boron
κ	particle or particle surface
æ	infinity
Note: uni	ts not stated, therefore any consistent set of units may be used
5.5 EDELM4	AN'S MODEL
A	number of moles of oxygen per mole of product
a	the total (dimensionless) particle consumption rate
В	number of moles of boron per mole of product
с _р	drag coefficient
ເ້	specific heat of the gas (ft ² /sec ² °K)
ເັ	specific heat of boron at the surface $(ft^2/sec^2 \circ K)$
ГS AH	heat of reaction (calorie/gram)
	surface reaction rate constant
L	latent heat of vaporization
M	molecular weight of boron (g/g·mole)
в M _{un}	molecular weight of nitrogen (q/q·mole)
NZ Mo	molecular weight of oxygen (q/g·mole)
⁰ 2	
^m prod	molecular weight of the product (g/g·mole)
ris D	average molecular weight at the particle surface (g/g·mole)
r	pressure (in almospheres)
^r v, B(T _p)	vapor pressure of boron (atm)
R	particle radius (feet)
T q	gas temperature (°K)
T_P	particle temperature (°K)
T _w	terperature of the wall ("K)
V _q	gas velocity (ft/sec)
	particle velocity (ft/sec)
8.5	mass fraction of boron at the surface of the particle
N ₂ ,S	mass fraction of nitrogen at the surface
'0,s	mass fraction of cxygen at the surface of the particle
′0 ₂ ,≖	mass fraction of oxygen in the surrounding (gas)

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Y prod.S	mass fraction of the product at the particle surface
a	fraction of vaporized product
δ _s	particle bulk density (slugs/ft ³)
C	emissivity
λ	the thermal conductivity of nitrogen (lbs force/sec °K)
Pq	gas density (slugs/ft ³)
P.	density at the surface of the particle (slugs/ft 3)
o	Stefan Boltzmann constant (lbs force/ft·sec °K ⁴)

and mass transfer. In most of the formulations the energy equation is the central element of the model, with the size history and other transport relationships representing auxiliary elements.

King (Refs. 11, 12) considers three stages in the boron combustion process: below the phase change temperature of the boron, at the point of boron phase change, and above the temperature at which phase change occurs (2450°K). Meese and Skifstad (Ref. 13), who based their model on King's 1972 paper (Ref. 12) also include boil-off of the oxide layer. In King's model it is assumed that the particle is moving at the velocity of the surrounding gas, while Meese and Skifstad and Edelman et al. allow for slip between particle and gas phase through the use of a convective heat transfer coefficient. Vovchuck (Ref. 14) does not include convective heat transfer, so that in Table 3 this section is omitted in summarizing Vovchuck's work. (A similar approach is followed in each case in which a given section of Table 3 does not apply to a particular model.) Particle-gas radiation is included in each of the models studied, and the expressions used in each model for this component of the overall heat transfer process are essentially interchangeable, with only those differences related to specific model geometry. It should be noted that the radiation term shown for Voychuk's model is eventually neglected.

King (Refs. 11 and 12), Meese and Skifstad (Ref. 13), and Mohan and Williams (Ref. 15) all consider oxide formation via the global reaction $B + 3/4 \ 0_2 + 1/2 \ B_2 \ 0_3$. Vovchuk (Ref. 14) allows for the formation of the lower oxides BO, BO₂, and B₂ 0_2 at the particle surface. Edelman el al. (Refs. 16, 17) considers the product species to be either BO or B₂ 0_3 , but if BO forms it does not oxidize further. Except for the work of Edelman, et al., all of the models assume that the reaction rate is diffusion controlled. The model described by Edelman, et al. involves a finiterate reaction of B to either BO or B₂ 0_3 (vapor). King, and Meese and Skifstad, both include oxide consumption in their models, through the effect of water on boric oxide ($B_2 \ 0_3 + H_2 \ 0 + 2 \ HBO_2$). The only other mechanism considered in any model for oxide removal is evaporation.

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The diffusion equations used in King's work are algebraic in form and depend upon the absolute value of the pressure at the surface and at infinity. Vovchuk integrates the partial pressure from the particle surface to infinity. For diffusion through the oxide layer King and Meese and Skifstad, use similar equations which vary only in one constant; the constant used by Meese and Skifstad was derived from data unavailable to King and thus provides a better fit of the available experimental data.

A major feature of King's model (Refs. 11, 12) is the expression representing boron phase change; Meese and Skifstad (Ref. 13) use a similar equation, derived, however, in a slightly different fashion. Edelman, el al. (Refs. 16, 17) provide an expression for the finite-rate evaporation of boron. Phase change does not directly enter the models reported by Vovchuk (Ref. 14) or Mohan and Williams (Ref. 15). King, and Meese and Skifstad, again use a similar expression for boric oxide evaporation, while Vovchuk, and Edelman, et al. have no oxide layer to remove. The oxide phase change model incorporated by Mohan and Williams instead of being equilibrium controlled, is finite rate. As noted earlier, Edelman, et al. describe the only model which includes finite-rate kinetics, but in this model it is assumed that the particle has ignited and no B_2O_3 layer is present, so that oxidation of the boron proceeds directly to either BO or B_2O_3 . Vovchuk considers only boron combustion but in the diffusion controlled mode.

The end product of Vovchuk's model is an expression for the particle burning time, and an expression for burning time is also obtained by Mohan and Williams. In the model described by Meese and Skifstad, it is assumed that no other phenomena occur while the oxide layer boils off, leading to an independent expression for the oxide layer boil-off time. All of the models except Vovchuk's provide expressions for the size decrease of the particle with time as combustion occurs; for those models which incorporate an oxide layer expressions for the time-rate of change of the oxide layer thickness are also defined by the analysis. In three of the models: those of King,

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Meese and Skifstad, and Mohan and Williams. ignition time is also provided. In each case ignition is defined as the point at which the oxide layer boils or flashes off.

What this review indicates is that the two most potentially useful models are those described by King (Refs. 11, 12) and by Edelman, et al. (Refs. 16, 17). Each of these approaches is the most general of its respective formulation; diffusion controlled burning in the King approach, including the effects of an oxide layer, and combined diffusion and finiterate kinetics, but without an oxide layer, on the model of Edelman, et al. The other approaches are either a derivative of these more general models or considerably more restricted in application.

Because it includes both diffusion and finite-rate chemical kinetics mechanisms, the model proposed by Edelman, et al. is useful for examining the available data for boron particle consumption rate as a function of particle size. Since the oxide layer is assumed not to exist, this approach can be interpreted as a model for the combustion process after particle ignition. It is thus useful for examining kinetics effects in boron consumption, keeping in mind that the results obtained represent a limiting case of the overall boron combustion process.

2.2.2 Model Description

The boron combustion model considered in this work involves the simultaneous solution of these coupled differential equations describing the velocity, size, and temperature of the particle. These equations can be written:

 $\frac{dV_p}{dt} = \frac{3C_p \rho_g (V_g - V_p)^2}{8R_\delta},$ (18)

where

C_D = drag coefficient P_g = gas density (slugs per cubic foot) V_g = gas velocity (ft/sec) V_p = particle velocity (ft/sec) R = particle radius (feet) δ_s = particle bulk density (slugs/ft³)

and

 $\frac{dR}{dt} = \frac{-a\lambda N_u}{2R\delta_s C_p},$ (19)

where

a = the total (dimensionless) particle consumption rate (see Eq. 21) λ = the thermal conductivity of nitrogen (in pounds force/sec °K) Nu = Nusselt number $C_{\rm p}$ = specific heat of the gas (in ft²/sec² °K), and the remaining

$$\frac{dT_{p}}{dt} = \frac{3a\lambda Nu}{2\delta_{3}C_{p_{s}}R^{2}C_{p}} \left[\frac{C_{p}(T_{g}-T_{p})}{e^{a}-1} - L + \frac{AK_{s}(2C_{p}\rho_{s}R)Y_{0_{2,s}}M_{B}\Delta H_{R}}{a\lambda NuM_{0_{2}}} - \frac{2o\epsilon RC_{p}(T_{p}^{4}-T_{w}^{4})}{a\lambda Nu} \right]$$
(20)

where

 c_{p_s} = specific heat of boron at the surface (ft²/sec² °K)

T_g = gas temperature (°K)

T_p = particle temperature (°K)

L = latent heat of vaporization

A = number of moles of oxygen per mole of product

K_s = surface reaction rate constant

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 P_s = density at the surface of the particle (slugs/ft³) $Y_{0_{2,s}}$ = mass fraction of oxygen at the surface of the particle M_B = molecular weight of boron (g/g·mole) ΔH_R = heat of reaction (calorie/gram) M_{0_2} = molecular weight of oxygen (g/g·mole)

σ = Stefan-Boltzmann Constant (lb.force/ft.sec °K⁴)
ε = emissivity
T = to set f the set of (0)

 T_w = temperature of the wall (°K)

and other parameters are as defined above.

The values for the remainder of the time-varying parameters are treated as simple algebraic equations (using the current value of T_n and R) as follows

$$a = \frac{88.662C_{p}\alpha R}{\lambda N u} \sqrt{\frac{M_{B}}{T_{p}}} \left[P_{v,B(T_{p})} - \frac{M_{s}}{M_{B}} Y_{B,s} P \right] + \frac{\frac{2M_{B}K_{s}Y_{0,s}C_{p}\rho_{s}RA}{M_{0,s}\lambda N u}}{\frac{M_{0,s}\lambda N u}{2}}$$
(21)

where

α

= fraction of vaporized product= vapor pressure of boron (atm)

PV,B(T_p) = vapor pressure of boron (atm)
M_s = average molecular weight at the particle surface (g/g·mole)
Y_{B,S} = mass fraction of boron at the surface of the particle
P = pressure (in atmospheres)

and other variables are as previously defined.



where $Y_{0_2,\infty}$ = mass fraction of oxygen in the surrounding (gas) B = number of moles of boron per mole of product and the remaining variables are as previously defined.

$$Y_{B,s} = (1-e^{-a}) \left[1 - AK_{s} \frac{2Y_{0_{2},s}C_{p}\rho_{s}R}{a\lambda Nu} \left(\frac{M_{B}}{M_{0_{2}}} \right) \right]$$
(23)
$$Y_{prod,s} = (1-e^{-a}) \left[\frac{2K_{s}Y_{0_{2},s}C_{p}\rho_{s}R}{a\lambda Nu} \left(\frac{M_{prod}}{M_{0_{2}}} \right) \right]$$
(24)

where Y prod,s = mass fraction of the product at the particle surface
M prod = molecular weight of the product g/g·mole)
and the remaining parameters are defined above

$$\tilde{M}_{s}$$
 = average molecular weight at the surface =
$$\begin{bmatrix} Y_{0}, s + \frac{Y_{B,s}}{M_{0}} + \frac{Y_{prod,s}}{M_{B}} + \frac{Y_{prod,s}}{M_{prod}} + \frac{Y_{N_{2,s}}}{M_{N_{2}}} \end{bmatrix}^{-1}$$

where M_{N_2} = molecular weight of nitrogen (g/g·mole)

i. D $Y_{N_2,s} = mass$ fraction of nitrogen at the surface and the remaining variables as previously defined.

$$Y_{N_2,s} = (1 - Y_{0_2,s} - Y_{B,s} - Y_{prod,s})$$
 (26)

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(22)

(25)

In this formulation the coupling is provided by the appearance in the energy equation of the parameter α , the total (dimensionless) particle combustion rate, which is itself a function of the surface concentrations of both $\mathbf{0}_2$ and B. Thus, the solution problem is one of solving three highly nonlinear, strongly coupled ordinary differential equations. The code developed for this work implemented a Newton-Raphson scheme to solve this coupled set of equations, and this approach proved to be reliable and relatively rapid. Thus the approach was then used to investigate different aspects of the combustion of boron through comparison of results with available experimental data.

2.2.3 Boron Combustion Analyses

The model described in this report combines both diffusive transport and chemical kinetic mechanisms and can thus be used to examine kinetics limitations on boron combustion as a function of particle size, ambient oxygen concentrations, pressure and ambient temperature. Each of these variables is of direct practical interest because each impacts the use of boron in a combustion process. For example, one strategy for maximizing boron combustion efficiency is to hold the boron in an oxygen-deficient environment until it is heated sufficiently to avoid oxide layer formation. Under this scenario, the kinetics of boron consumption at elevated gas temperatures becomes important. As another example, in many propulsion system applications a boron-slurry-fueled vehicle would be required to operate over a wide range of altitudes and flight Mach numbers. This impacts both the temperature in the combustor and the ambient pressure. Thus, these impacts on the kinetics of boron consumption are of interest.

As particle size decreases, at constant pressure, the effects of chemical kinetics increase relative to those of diffusion. This is clearly shown by the results presented in Fig. 16. For cxample, for 1 atm pressure, the transition from kinetics control ($\tau_b \approx d$) to diffusion control ($\tau_b \approx d^2$) occurs for particles somewhat larger than 200 µm. However, this transition

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Figure 16. Predicted Kinetic-to-Diffusion Controlled Combustion of Boron

is itself a function of pressure, as the results indicated in Fig. 16 also show. At low pressure, typical of high-altitude ramjet operation, the transition to diffusion control occurs at diameters so large as to be well outside the range of practical interest (for this hot-gas, hot particle case), while at high pressures, such as might be encountered in an advanced gas turbine combustor, the consumption process is diffusion-controlled even for quite small particles.

In most applications, boron particle sizes must be kept small, even at elevated pressures, to avoid long burn times. This is illustrated by Fig. 17, in which the results depicted on Fig. 16 are cross-plotted to indicate the effects of pressure on consumption time for a given particle size. It is immediately evident from this figure that for large particle sizes burn times greater than 10 ms would be expected (in the absence of a B_2O_3 coating; considerably larger burn times can be anticipated for B_2O_3 -clad particles). Note also that for large particles the burn time tends to become independent of pressure at high pressures as the transition to diffusion control is completed. For small particles, on the other hand, kinetics effects dominate throughout the pressure range studied, and at a few atmospheres pressure burn times of a fraction of a millisecond can be achieved.

While the data shown in Fig. 16 represent high-temperature boron combustion, much of the available data involves ignition and combustion in a cold environment. Figs. 18 and 19 provide data at several pressure levels, for several particle sizes, at two ambient oxygen concentrations, and show comparisons between the data and predictions carried out using the present model. Overall, the agreement between the data and the model predictions is quite good, although the model does not represent well the decrease in burn time at pressures above about 20 atmospheres that may be indicated by the data. Another aspect of the model prediction is also of interest: at low pressures, for smaller particles, the model predicts that the boron consumption process will quench, leaving a non-negligible residue. This residue particle, while not insignificant from a combustion inefficiency standpoint,

-62-



1.4

Figure 17. Effect of Pressure on Burn Time



Figure 18. Comparison of Predictions with Data; Oxygen Concentration = 0.21, T_{Gas} = 300°K

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Figure 19. Comparison of Predictions with Data: Oxygen Concentration = 0.40, T_{Gas} = 300°K

is not large and could be missed in experimental studies unless its presence was specifically being investigated. The quenching process appears to occur at high pressures for smaller particles, and could be of considerable significance in ramjet operation, where afterburning can be continuing in the exhaust nozzle.

2.2.4 Finite-Rate B203 Condensation

While the existence of B_2O_3 as an oxide coating on a boron particle is of critical importance in the examination of boron particle ignition, the <u>condensation</u> of the oxide out of the gas phase is also critical to the overall performance of a boron slurry fueled ramjet. This follows from the fact that approximately 30% of the available energy of boron combustion is tied up in the phase transformation between liquid and gaseous B_2O_3 . Where recondensation of B_2O_3 occurs -- in the combustor or in the nozzle -- is thus critical to achieving the optimum performance levels utilizing boron fuels.

Finite-rate condensation effects can be analyzed using single particle nucleation and growth theory. For example, nucleation rate can be approximately using the expression

$$J = \text{Bexp}\left(\frac{-\Delta G}{KT}\right)$$
(27)

from classsical kinetic theory, where

K is the Boltzmann constant, T is the local temperature, and B is a rate constant;

 ΔG is the free energy of formation of a critical cluster, itself a function of the surface tension of the material, the work of cluster formation, and the number of molecules in a critical droplet. Thus $\Delta G \approx f_1$ (σ , ω^* , n^*). w*

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and n^* are both functions of r^* , where r^* is the radius of a critical droplet A number of expressions have been devised for the terms representing the work of cluster formation and the number of molecules in a critical droplet. For example, in the expression developed by Yang (Ref. 18) and used by Edelman and Economos (Ref. 19) to examine boron condensation phenomena, the work of cluster formation is given by

$$\omega \star = \frac{4}{3} \pi \sigma r \star^2 \tag{28}$$

where σ is the liquid surface tension, and the number of molecules in a critical drop is expressed as

$$n^{*} = \frac{4}{3} \pi \frac{r_{\star}^{*3}}{M_{l}} \zeta_{L}$$
 (29)

in which M_{L} is the molecular weight and G_{L} the density of the liquid condensate.

The radius of a critical drop can be expressed as

$$r^{*} = \zeta_{L} \frac{R_{O} T \ln (P_{V} / P_{V_{\infty}})}{(30)}$$

where P_v is the vapor partial pressure and $P_{v\infty}$ is the equilibrium-saturation partial pressure, i.e., the vapor pressure of a vapor in equilibrium with a plane surface of condensed phase. R_o is of course the universal gas constant.

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Once the nucleation process produces a critical size droplet, it continues to grow by the additional deposition of condensing vapor. A growth law which has been used to calculate water vapor condensation phenomena is given by the expression

$$\frac{d\mathbf{r}}{dt} = \frac{\left(\mathbf{P}_{\mathbf{v}} - \mathbf{P}_{\mathbf{v}_{\infty}}\right)}{\zeta_{L}} \left(\frac{M_{L}}{2\pi K t}\right)^{1/2}$$
(31)

Finally, the total production rate of condensed-phase B_2O_3 can be written

$$\dot{w}_{B_2 0_3} = \dot{w}_n + \dot{w}_G = \rho J + \sum_{j} w_p j \qquad (32)$$

where the growth rate term is summed over several classes of particles defined by a mean radius r_i , i.e.,

$$w_{p}^{j} = 4\pi (r^{j})^{2} \rho_{L} N_{p}^{j} \frac{dr^{j}}{dt}$$
(33)

in which $N_p^{\ j}$ gives the number density of particles of radius class j.

Application of this approach to the finite-rate condensation of B_2O_3 requires knowledge of the surface tension of B_2O_3 and its equilibrium-saturation partial pressure. These data can be estimated for the temperature ranges of interest through modest extrapolation of available data. For example, as shown by Fig. 20, data included in the JANNAF tables allows a modest extrapolation of the low-temperature data to fit the empirical expression

$$P_{V_{\infty}} = \exp\left(19.03 - \frac{44080}{T}\right)$$
 (34)

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Figure 20. B₂O₃ Vapor Pressure Data

Surface tension data requires a rather larger extrapolation, as shown by the data included in Fig. 21.

The physical data described here and the expressions for nucleation and condensation set out in this section were used in the work outlined in Ref. 19 to compute the condensation of B_2O_3 in a supersonic nozzle expansion process; the B_2O_3 condensation model was incorporated in an analysis which coupled finite-rate chemistry for the B-O-H-N system with finite-rate condensation phenomena. Fig. 22 shows the nozzle pressure distribution data obtained in a test involving B_2O_3 condensation. These experimental data show a definite departure from the otherwise isentropic expansion associated with the conical nozzle geometry. Also given in this figure are the results of a calculation based on the assumption that the latent heat of B_2O_3 condensation is released instantaneously, resulting in a Rayleigh line process assumed to occur in the vicinity of the condensation-induced pressure rise as indicated by the data. The heat release used in the Rayleigh model is based on the condensation of all of the available B_2O_3 in the flow. These results indicate that the agreement of the Rayleigh analysis and the experimental data is in fact quite good, although the ideal model somewhat overestimates the magnitude of the experimental pressure rise. On the other hand, the coupled finite-rate condensation and gas phase kinetics approach agrees fairly well with the data though the initial pressure change is somewhat underpredicted. This initial underprediction casts some doubt on the nucleation and growth laws used in this study, but given the meager data available both for the physical parameters which enter the models and for testing and development of the expressions themselves, such a deviation from measured data as shown here is not unexpected. This work does, on the other hand, provide evidence that the effects of $B_2^{0}O_3$ condensation can be included in analytical approaches intended to model the performance of boronfueled combustors.

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Figure 21. Surface Tension of B_2O_3





2.2.5 Discussion

The results presented in this section indicate that a coupled diffusion and finite-rate kinetics approach is required to adequately examine boron combustion in the context of its use as a fuel in ramjet combustors. These results show that coupling finite-rate oxidation kinetics with diffusional processes allows the behavior of boron combustion as observed in laboratory experiments to be explained, in terms of burn time/particle size and pressure and temperature relationships. An understanding of these phenomena is crucial to the utilization of boron in combustors. The computations also clearly indicate quenching of the boron combustion process even for clean (oxide free) particles for certain combinations of partical size, ambient temperature, and ambient oxygen concentration.

Just as clearly the work described herein indicates the need for a number of improvements. For example, incorporation in the modeling of the presence of an oxide layer on the particle is needed to adequately account for boron ignition phenomena. The role and potential importance of suboxide formation and disposition remains unclear, and more mechanistic and detailed models of B-O, B-O-H, and B-O-H-C kinetics are clearly required. Additionally, the work reported herein also shows that B203 condensation processes can be modeled, and the impact of this on the overall heat release obtained with boron combustion is such that B_2O_3 condensation needs to be controlled to optimize combustion efficiency. Further work remains to establish appropriate analyses of these processes. Finally, cloud and slurry spray combustion analyses need to be established to aid in the practical use of boron slurry fuels. The individual parts of such an analysis exist, as indicated by the spray modeling work considered in the preceding section, the single-particle boron modeling considered here, and the modular model work to be discussed in the next section. What is required is the merging of the efforts in these three research areas.

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2.3 THE MODULAR MODEL FOR RAMJET PERFORMANCE ASSESSMENT

The modular model for ramjet performance assessment represents the most advanced and detailed combustor model applicable to suddenexpansion ramjets. It has been developed because the complex flame stabilization, flame propagation, and spray combustion problems which have been encountered in the development of dump combustors require a detailed analytical capability for their resolution. 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.

In its basic form, the modular model approach has been described in a variety of reports and papers, of which Refs. 20 and 21 are examples. The model described in this report, however, differs from those previously described in two key areas: first, the well-stirred reactor chemistry model is fully integrated with the chemistry modeling applied to the directed flow, and second, the advanced quasiglobal model for hydrocarbon combustion kinetics is incorporated in the code. This latter difference between the present model and prior versions of the modular approach is extremely important because it is only with the advanced quasiglobal model that it is possible to accurately characterize the combustion kinetics and heat release processes that occur in fuel-rich regions. Since fuel-rich regions make up a significant portion of nonpremixed ramjet combustor flowfields, and can be a significant cause of combustion inefficiency in ramjet operation, this fuel-rich combustion characterization ability is a key requirement for an overall ramjet combustor performance mod 1.

The modular concept is that the combustor flowfield can be broken down into three major components, as repre erfed schematically in Fig. 23. These components are a directed flow (which is computationally modeled as a flowfield satisfying the boundary layer approximation that axial gradients are negligible compared to radial gradients, and the static pressure is radially uniform); a recirculation zone (assumed to be representable as a well-stirred reactor or a combination of well-stirred reactors); and a turbulent shear layer region, located along the dividing Streamline

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Figure 23. Schematic of Sudden-Expansion (Dump) Burner

 which separates the other two regions. The shear layer serves to couple the other two model components; fluxes of species and energy across this shear layer form the boundary conditions on the two computational regions. The directed flow is assumed to be fully turbulent, with the turbulent effective viscosity defined by a conventional two-equation turbulence model (Ref. 22).

2.3.1 <u>Stirred Reactor Modeling of Dump Combustor Recirculation Zones</u>

The well-stirred reactor, shown schematically in Fig. 24, 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 flow, $\rho V/\dot{M}$; 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, which allows the use of rapid and efficient solution procedures.

In the lower half of Fig. 24, 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. 24(b) is similar to the volume within the laboratory stirred reactor in Fig. 24(a), and the same solution technique can be used to obtain the thermo chemical static. A comparison of Figs. 24(a) and 24(b) 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

-76-



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a)



Figure 24. Comparison of Well-Stirred Reactor with Recirculation Region Flowfield.
a) Schematic design of Spherical Well-Stirred Reactor
b) Schematic of Sudden-Expansion Recirculation Region

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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 streamline, 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:

$$\begin{array}{ccc} \text{Continuity} & \overset{\bullet}{\mathbf{m}}^{\mathbf{I}} = \overset{\bullet}{\mathbf{m}}^{\mathbf{O}} = \overset{\bullet}{\mathbf{m}} \end{array}$$
 (35)

Species,

ĺ

$$\frac{dM\alpha_{i}}{dt} = m_{i}^{I} + V w_{i}$$
(36)

 $h = \sum_{i} h_{i} \alpha_{i} = h^{I} + \dot{Q}/\dot{m}$ Energy, (37)

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 $d\alpha_i/dt \rightarrow 0.$

Equations (35-37), 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.

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$$-2\pi \int_{0}^{s} R_{c}(X) \rho v_{T} \sum \left[h_{i}^{I} (T^{I}) \frac{\partial \alpha_{i}^{I}}{\partial r} \right] ds + \dot{Q}$$

$$= 2\pi \int_{0}^{s} R_{c}(X) \kappa \frac{\partial T}{\partial s} ds \qquad (38)$$

$$-2\pi \int_{0}^{s} R_{c}(X) \rho v_{T} \sum_{i} \left[h_{i}^{0} (T_{R}) \frac{\partial \alpha_{i}^{0}}{\partial r} \right] ds$$

and

$$\frac{d\alpha_{i}}{dt} = \frac{-2\pi}{\rho_{c}V} \int_{0}^{s} R_{c}(X) \left[\rho v_{T} \frac{\partial \alpha_{i}}{\partial r}\right] ds$$
$$- \frac{2\pi}{\rho_{c}V} \int_{0}^{s} R_{c}(X) \left[\rho v_{T} \frac{\partial \alpha_{i}^{0}}{\partial r}\right] ds + \frac{\dot{w}_{i}}{\rho_{c}}$$
(39)

where ρv_T is evaluated using the outer flowfield solution in the region of the dividing streamline.

Because in the modular model one 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

$$\begin{pmatrix} \hat{\sigma}\phi \\ \hat{\sigma}r \end{pmatrix}_{W} = \frac{\phi_{P} - \phi_{R}}{1}$$
(40)

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

$$l = ax + b \tag{41}$$

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 to be relatively insensitive to the values of the coefficients a and b in Eq. (41); for the results presented in this report, a = 0.03 and b = 0.07.

2.3.2 Parabolic Mixing: The Director-Flow Model

The second major element of the modular model for a suddenexpansion 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,

$$\frac{\partial r \rho u}{\partial x} + \frac{\partial r \rho v}{\partial r} = 0 \tag{42}$$

Species Diffusion for the ith Specie,

$$\rho u \frac{\partial \alpha_{i}}{\partial x} + \rho v \frac{\partial \alpha_{i}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \rho \frac{v_{T}}{Sc} \left[\frac{\partial \alpha_{i}}{\partial r} \right] \right\} + \dot{w}_{i} \qquad (43)$$

Momentum Equation,

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \rho v_T \frac{\partial u}{\partial r} \right) \right\} - \frac{\partial p}{\partial x}$$
(44)

Energy Equation,

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left\{ \frac{r \rho v}{Pr} \int_{c} \left[\frac{\partial H}{\partial r} - \left(\frac{Pr}{Sc} - 1 \right) \right] \right\}$$

$$\sum_{i} h_{i} \frac{\partial \alpha_{i}}{\partial r} + (Pr - 1) \frac{\partial}{\partial r} \left(\frac{u^{2}}{2} \right) \right]$$
(45)

These equations, along with expressions for the enthalpy

$$H = h + (u^2/2)$$
 and $h = \sum_{i} \alpha_i h_i(T)$ (46)

and the equation of state

$$p = \rho RT \sum_{i} (\alpha_{i}^{\prime}/W_{i})$$
(47)

can be solved, given an expression for the turbulent eddy viscosity $\mu_T = \rho v_T$. This is defined by a two-equation turbulent kinetic energy model, 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

$$\rho u \frac{\partial k}{\partial x} + \rho v \frac{\partial k}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\mu_T r}{\sigma_k} \frac{\partial k}{\partial r} \right) + \mu_T \left(\frac{\partial u}{\partial r} \right)^2 - \rho \epsilon$$
(48)

Turbulence Energy Dissipation,

$$pu \frac{\partial \varepsilon}{\partial x} + pv \frac{\partial \varepsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\mu_T r}{\sigma_k} \frac{\partial \varepsilon}{\partial r} \right) + C_{E1} \frac{\varepsilon}{k} \mu_T \left(\frac{\partial u}{\partial r} \right)^2 - C_{E2} p \frac{\varepsilon^2}{k}$$
(49)

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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 described in this report: thus $C_{\mu} = 0.09$. $C_{E1} = 1.40$, $C_{E2} = 1.95$, $\sigma_k = 1.00$, and $\sigma_{\epsilon} = 1.22$.

2.3.3 Chemical Kinetics: The Advanced Quasiglobal Model

It has long been noted that an important limitation of the original basic quasiglobal formulation is its inapplicability under fuel-rich conditions; e g., for fuel-air ratios greater than stoichiometric. For equivalence ratios greater than about 1.5, the adiabatic flame temperature predicted by the basic quasiglobal approach is greater than that observed in experiments, and the discrepancy between the predicted and measured adiabatic flame temperatures becomes larger as the combustion process becomes more fuel-rich. This is a serious difficulty with respect to diffusion flames in general and in liquid-fueled sudden-expansion combustor ramjet applications in particular. In these devices the local fuel-air ratio in and near the flame-stabilizing recirculation regions has been found to be well above stoichiometric. Gas turbines as well often have fuel-rich primary zones in their combustion chambers. Thus a clear need exists for an improved quasiglobal model, in order to examine kinetic processes in fuel-rich combustor regions.

The basic reason that the original quasiglobal model formulation fails in the prediction of combustion processes in fuel-rich regions is that it does not include the fuel pyrolysis steps that occur in high temperature, oxygen deficient regions, but instead assumes a pure oxidation step for fuel consumption. In the fuel rich regions, both pure pyrolysis and oxidative pyrolysis steps occur to lead to the breakdown of the fuel into lower molecular weight components. At the same time, soot formation occurs: while this process does not soak up a large amount of energy, it does result in the formation of particulates that strongly increase the radiative heat loss from the flame. This radiation enhancement results in both a decrease in the overall temperature (and thus can directly affect the rate of heat release) and an increase in the heat load to the combustor walls. Eased on these observations, the advanced quasiglobal model incorporates both fuel pyrolysis and soot formation steps.

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In the advanced quasiglobal kinetics approach, the fuel to be modeled is broken down into aromatic and aliphatic components: soot formation is dependent on the amount of aromatic fuel present. The aromatic and aliphatic components are modeled using rates which have been developed for toluene and iso-octane, respectively. That is, the model fuel component which can be treated as aromatic is assigned rates which have been developed by extensive comparison of toluene predictions with experimental data, and the model fuel component that can be treated as aliphatic is assigned the rates developed for iso-octane. Each of these fuels break down into secondary fuels, C_2H_2 from toluene and C_2H_4 from iso-octane, following the pure pyrolysis pathway, as well as partially oxidizing by attack from both O_2 and OH. The secondary fuels then react with the remaining OH and O_2 , and the wet CO mechanism follows. Table 6 illustrates these reactions, along with soot formation/consumption reaction.

While this remains a formidable list of reactions, our studies show that the accuracy of the predictions is most sensitive to the wet-CO portion of the mechanism. This observation indicates that further simplifications are possible depending on the information being sought. For example, Table 7 shows a simplified mechanism intended to examine the heat release distribution in a ramjet combustor where the flame is stabilized by a recirculation zone. In this example, many of the intermediates important in a lower temperature ignition process are presumed to be negligible because of the presence of the recirculation zone. Also, in this example the fuel, JP-7, has been modeled as $C_{12}H_{24}$, and has been treated as being aliphatic in character.

2.3.4 Fuel Injection Model

In addition to the basic components of a parabolic, directed flow analysis and a well-stirred reactor formulation, the modular concept includes other elements of the dump combustor flowfield, for example, the fuel injection process. The detail of the computation provided by the use

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TABLE	6.	TOLUENE	AND	ISO-OCTANE	OUAS1GLOBAL
		KINETICS	s moe)EL	

GLOBAL MECHANISM	1 A	1 8	E/R	POWER DEPENDENCIES	
	1				
Toluene (aromatic)				1	
C ₂ H ₂	1.7987 E10	0	3.5000 E4	{C ₇ H ₈ } ^{1.0}	
С ₇ н _а + 3.5 0 ₂ 7 со + 4 н ₂	4.4963 89	1 .	2.6785 E4	[C,H,)0.5(0,)1.0	
$C_7H_8 + 0H - 3.25 C_2H_2 + 0.5 C0 + 0.5 H_20 + 0.75 H_2$	1.4721 E17	0	1.4510 E4	{с ₂ н ₈ } ^{1.0} (он) ^{1.0}	
Iso-Octane (aliphatic)		1			
C ₈ H ₁₈ 4 C ₂ H ₄ + H ₂	1.0473 E12	0	3.5229 E3	[C8H18]1-0	
с _в н ₁₈ + 4 0 ₂ 8 со + 9 н ₂	1.2900 E9	1	2.5160 E4	[C8H18]0.5[02]1-0	
· _B H _{1B} + 0H3.75 C ₂ H ₄ + 0.5 C0 + 0.5 H ₂ 0 + 1.5 H ₂	2.000 E17	0	1,4919 E4	[с ₈ н ₁₈ [^{1.0} [он] ^{1.0}	
Secondary Fuel	•				
$C_{1}H_{1} + 6 OH - 4 H_{2}O + 2 CO$	4.7850 E15	0] 1.3883 £4 t	[С.н.] ^{1.0} [он] ^{1.0}	
$C_{nH_{n}} + 2 \text{ OH} \rightarrow 2 \text{ CO} + 2 \text{ H}_{n}$	2.8000 E16	0	0	[C_H_] ^{1.0} [OH] ^{1.5}	
$C_{0}H_{4} + 6 \text{ DH} \longrightarrow 2 \text{ CO} + 2 \text{ H}_{0} + \text{H}_{0}$	2.2020 E15	0	1.2079 E4	[C_H_] ^{1.0} [OH] ^{1.0}	
$C_{2}H_{4} + 2 \text{ OH} \longrightarrow 2 \text{ CD} + 3 \text{ H}_{2}$	1 2.1129 E27	-3.0	6.3062 E3	[C_H_] ^{1.0} [OH] ^{1.5}	
2 4 2 C,H, + O, = 2 CHO	4.0000 E12	0	1.4092 84	[C_H_] ^{1.0} [0_] ^{1.0}	
$c_2H_4 + M = c_2H_2 + H_2 + M$	 2.0293 E17 	0 1	3.9810 E4	[с ₂ н ₄] ^{1.0} [н] ^{1.0}	
Soot Reactions			1		
C ₇ H ₈ = HC -→ soot	-4.0465 E14*	-2.0	1.6110 E4	[HC] ^{}.43} [0 ₂] ^{-0.5}	
soot + 0 ₂ C0 ₂	[soot] = -	^{12 P} 02 ^A t	$\int \frac{\kappa_A x}{1 + \kappa_7 p_0} dx$	κ _B ^(1-χ)	
$x = \left[1 + \kappa_{T} \times \left(\kappa_{B} P_{O_{2}}\right)\right]^{-T}$					
$K_i = A_i \exp \left\{-E_i / RT\right\}, i = A, B, T, Z$					
1 = A B T Z	2.000 E1 (4.4600 E-3) 1.5100 E5 (2.1360 F1		1.5090 E4 7.6490 E3 4.8820 E4 2.0630 F3	As indicated by the equation for [soot]	
where $A_{\rm E} + 6 (C_{\rm g}/\rho_{\rm E} + D_{\rm g}) (cm^2 surface/cm)$	3), P_{0} = parts	al pressu	re of O ₂ (atm)		
$C_{-} = (g + soot/cm^3 of cas), \rho_{-} = (c_{-})$	_2 • ±:ct/cm ³ of €	oot), D	- • disater of -	soot (cm).	
[scot] = mass of soct/volume of cas (o/er	n ³).	5			

TABLE 6. (Continued)

ELEMENTARY MECHANISM			
	A	B	E/R
HE Fragmentation Mechanism		1	
CH4 + DH = H50 + CH3	3.0000 E13	j I O	1 3020.0
Ч 2 3 СН _а + 0 = ОН + СН _а	2.0000 E13	 0 ·	1 4640.0
CH _A + H = H ₂ + CH ₃	1.2600 E14	0	 598 9.0
CH3 + 0 = H + HCH0	1.3000 E14	0	1 1006.0
CH ₁ + 0 ₂ = OH + HCHO	1.7000 E 12	D	7045.0
сн _р . н = Н _р + Сн	2.5210 E11	0.67	12934.1
$CH_2 + OH = H_2O + Ch$	2.5120 E11	D.67	12934.1
СH ₂ + 0 ₂ = ОН + СНО	1.0000 E14	0	1862.0
сн + 0 ₂ = 0 + сно	1.0000 E13	0	D
сн + со ₂ = со + сно	1.0000 E10	0.5	2.0000 E3
Сн + он = н + сно	5.0000 E11	0.5	5.0000 E3
CH + O = H + 20	5.0000 E11	0.5	1 0
CH ₄ + M = H + CH ₃ + M	4.0000 E17	0	44500.0
$CH_3 + H = CH_2 + H_2$	2.0000 E11	0.7	1 1510.0
сн ₃ + он + сн ₂ + н ₂ о	6.0000 E10	0.7	 1010.0
Wet CO Mechanism			
$H_2 + 0_2 = 0H + 0H$	1.7000 E13	0	2.407D E4
$OH + H_2 = H_2O + H$	2.1900 E13	o	2.5900 E3
$0H + 0H = 0 + H_20$	6.0230 E12	0	5.5000 E2
0 + H ₂ ± H + ОН	1.8000 E10	1.0	4.4800 E3
$H + 0_2 = 0 + 0H$	1.2200 E17	-0.91	8.3690 E3
2 M + O + H = DH + M	1.0000 E16	1 0	0
$M + 0 + 0 = 0_2 + M$	2.5500 E18	-1.0	5.9390 E4
с М + H + H = H ₂ + М	5.0000 E15		0
м + н + он = н ₂ о + м	8.4000 E21	-2.0	0
CO + OH = H + CO,	1 4.0000 E12		4.0300 E3
	1		2 5.050 54
$c_{0} + 0_{j} = (0_{j} + 0_{j})$	3.0000 E12		1.5000 14

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TABLE 6. (Continued)

A	В	E/R
	1	! !
3.0000 E13	0	0
1.7000 E13	0	1.5100 E3
3.0000 E13	0	0
3.0000 E13	0	0
1.0000 E14	0	0
1.2600 E14	0	0
1.0000 E12	0	4.0300 E3
1.0000 E14) 0 -	1.5100 E3
3.1620 E12	0	3.5230 E3
5.0120 E16	o	3.6740 E4
5.0000 E14	о [.]	9.5620 E3
1 2600 517		2 2000 64
		2.2300 [4
3.9800 E13		2,1440 24
1.5850 E12		1.9120 23
1.0000 E13		9.0600 EZ
5.0100 E13	0	5.0300 EZ
5.0100 E13	0	5.0300 E2
2.5000 E14	D I	9.5630 E2
2.5100 E13	0	3.5230 E2
1.5800 £15	0	-5.0340 E2
1.0000 E10	0	o
	A 3.0000 E13 1.7000 E13 3.0000 E13 3.0000 E13 1.0000 E14 1.2600 E14 1.0000 E14 3.1620 E12 5.0120 E16 5.0000 E14 1.2600 E17 3.9800 E13 1.5850 E12 1.0000 E13 5.0100 E13 5.0100 E13 5.0100 E13 5.0100 E13 1.5800 E15 1.6000 E10	A B 3.0000 E13 0 1.7000 E13 0 3.0000 E13 0 3.0000 E13 0 1.0000 E13 0 1.0000 E14 0 1.2600 E14 0 1.0000 E12 0 1.0000 E14 0 3.1620 E12 0 1.0000 E14 0 3.1620 E12 0 5.0120 E16 0 5.0120 E16 0 1.2600 E17 0 3.9800 E13 0 1.5850 E12 0 1.0000 E13 0 5.0100 E13 0 5.0100 E13 0 2.5000 E14 0 2.5000 E13 0 2.5000 E14 0 1.5800 E15 0 1.0000 E10 0

M indicates general third body.

GLOBAL MECHANISM		1 8	E/R	POWER DEPENDENCIES
Primary Fuel			 	1
C ₁₂ H ₂₄ 6 C ₂ H ₄	1.0473 E12	0	3.5229 E4	(c _{12^H24}) ^{1.0}
$C_{12}H_{24} + 6 O_2 - 12 CO + 12 H_2$	1.2900 89	1	2.5164 E4	[C ₁₂ H ₂₄] ^{0.5} [0 ₂] ^{1.0}
$C_{12}H_{24} + DH - 5.75 C_2H_4 + 0.5 CO + 0.5 H_2O + 0.5 H_2$	2.0000 E17		1.4919 E4	[{C ₁₂ H ₂₄] ^{1.0} [ОН] ^{1.0}
Stcondary Fuel	1 		1	
C2H4 6 0H 2 CO + 4 H20 + H2	2.2020 E16	0	1.2079 E4	[с ₂ н ₄] ^{1.0} [он] ^{1.0}
C2H4 + 2 0H 2 CO + 3 H2	2.1129 E27	-3	6.3062 E4	[с ₂ н ₄] ^{1.0} [он] ^{1.5}
C2H2 + 6 0H 4 H20 + 2 CO	4.7850 E15	1 0	1.3883 E4	[[2H2]]1.0[OH]1.0
C ₂ H ₂ + 2 OH 2 CO + 2 H ₂	2.8000 E16	0	0.0	[c ₂ H ₂] ^{1.0} [он] ^{1.5}

TABLE 7. FINITE RATE KINETICS MODEL USED IN RAMJET COMPUTATIONS

ELEMENTARY MECHANISM	A	B	£/R	1
Wet CD Mechanism	1	1		
со + он = н + со ₂	4.0000 E12	0.0	4.0260 E4	
он + н ₂ = н ₂ о + н	2.1900 E13	0.0	2.5900 E4	
Он + ОН = 0 + Н ₂ 0	6.0230 E12	0.0	5.5000 E2	
0 + H ₂ = H + OH	1.8000 [11	1.0	4.4800 E3	
$H + 0_2 = 0 + 0H$	1.2200 E17	-0.91	8.3690 E3	
0 ₂ + H ₂ = 0H + 0H	1.7000 E13	0.0	2.4070 E4	
$c_0 + o_2 = 0 + c_00$	3.0000 E12	0.0	2.5000 E4	
C + H = OH + M	1.0000 E16	0.0	0.0	
В + Н = Н ₂ + М	5.0000 E15	0.0	0.0	
н • сн = н ₂ 0 + м	8.4000 t21	-2.0	0.0	
$CO + O = CO_2 + M$	E.0000 E13	0.0	0.0	
M + C ₂ = 0 + 0	2.5500 t18	-1.0	5.9386 E4	
$M + C_2 H_4 = H_2 + C_2 H_2 + M_1$	2.0983 E17	0.0	3.9810 E4	
	1	• !		

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of a parabolic directed flow analysis is the key feature of the modular model that allows the inclusion of a fuel injection module. This is particularly true in the case of liquid fuel injection, for at the fuel/air ratios appropriate for ramjet combustor operation, the liquid fuel streams initially occupy a very small portion of the overall combustor crosssectional area. The liquid fuel injection model makes use of a combination of empirical information and turbulent mixing calculations. For example, the fuel jet penetration from the wall is computed through the use of an empirical penetration correlation (Ref. 23), using a breakup time correlation (Ref. 24) to estimate the downstream distance at which penetration is to be computed. That is, it is assumed that the fuel jet has turned parallel to the airflow at the axial position at which the initial fuel jet has broken up into droplets, as given by the breakup time correlation and the local airflow velocity.

Since the basic modular model formulation involves an axisymmetric flowfield, individual fuel jets cannot be resolved, and it is assumed that the liquid fuel spray forms an annulus whose cross-sectional area may either be specified or computed based on an assumed fuel spray bulk velocity. A bulk spray evaporation correlation is then used to compute the fuel vaporization rate; this correlation (Ref. 25) is a function of the initial velocity and temperature difference between the fuel spray and the surrounding air stream. Spreading of the fuel jet is computed through use of a turbulent mixing hypothesis as for the mixing process in the remainder of the parabolic flow. Fig. 25 shows the results of a computation of the fuel injection process for three fuel injectors, located in the combustor inlet wall, along with the centerline, and in a midstream position. Shown are the computed contours of the fuel mass fraction, α_F , with the vapor-phase fuel shown as the solid line and the liquid-phase fuel as the dotted line, as a function of both axial and radial position in the combustor inlet. For these calculations the air inlet velocity was approximately 700 ft/sec at a temperature of 1600°K; the overall fuel/air equivalence ratio was 0.6. The results shown in Fig. 25 provide a good example of the detail of the fuel injection process available through use of this aspect of modular modeling.

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2.3.5 Iteration Procedure

The overall logic of the calculation procedure is shown schematically in Fig. 26. Inlet conditions can be defined upstream or downstream of the fuel injection station as required; if liquid fuel injection is specified, the penetration and spreading of the liquid fuel jets are computed as described in the preceding section. The computation proceeds to the dump plane in the sudden-expansion combustor, at which point the dependent variables in the flowfield are stored for later use in the recirculation zone iteration procedure.

An initial state of the stirred reactor must be specified in order to begin the iteration procedure. This state is reasonably arbitrary, except that a reacted temperature level must be specified. The shape of the dividing streamline separating the directed flow and the recirculation zone must also be specified, along with the shear stress level, expressed as a "skin friction" coefficient. The initial stirred reactor state, in conjunction with a model for the shear layer between the recirculation zone and the directed flow then defines the boundary conditions for the parabolic directed flow calculation. Directed flow computations are carried out to the axial station at which the end of the recirculation zone has been defined; as part of these computations the diffusive flux of species and energy across the dividing streamline is computed. These fluxes then define a new set of stirred reactor "feed rates," i.e., species and energy fluxes into the recirculation zone region. Convergence of the procedure is defined by the change in the stirred reactor feed rates from iteration to iteration; each species and the energy flux must change less than 1.0% before the convergen e criteria are satisfied. If they are not, the species and energy fluxes, and the overall diffusive mass flux and physical recirculation zone volume are used to compute a new stirred reactor state. The pressure required for this computation is taken to be the arithmetic average of the pressures computed as part of the directed flow solution at the beginning and end of the recirculation region. The new stirred reactor state is then used to define the directed flow boundary conditions, and the computation is restarted from the

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dump station. When convergence is achieved, typically in 3-5 iterations, the combustor calculation is continued to the specified combustor exit station.

2.3.6 Modular Model Assessment

A variety of applications of different versions of the modular model have been reported in the literature, Refs. 20 and 21, and performance calculations have been carried out for several types of sudden expansion ramjet combustors, with inlet conditions including premixed, uniform inlet profiles, wall and in-stream orifice fuel injectors, and wall-mounted poppet type fuel injectors.

An early set of modular model validation comparisons included the sudden expansion ramjet combustor results described by Craig, et al. (Ref. 26). This work involved a combustor L/D of 3, a dump area ratio A_3/A_2 of 2.25, and an exit nozzle area ratio $A_2/A_3 = 0.40$. Cold flow and reacting flow experimental results are both the reported for this configuration. In the modular model computations, the cold flow data were used to evaluate the model coefficient values for the specific configuration, and computations of a premixed dump combustor at a fuel/air ratio of 0.053 were then carried out using these coefficient values for comparison with the data presented in Ref. 26. In the experiments, the fuel used was JP-4 which was represented in the computations by propane. Both a simple one-step global finite-rate chemistry model and the full hydrocarbon oxidation kinetics as represented by the quasiglobal model were used to represent the chemical kinetics processes in the directed flow. A global model was used for the recirculation zone in all cases. Propane was chosen to represent the fuel because it adequately simulates from a heat-release standpoint the actual fuel used and because previous studies with propane had resulted in the development of a one-step finite-rate kinetics model for this fuel. This one-step model represents fairly accurately the ignition delay for propane-air (although not the overall reaction time) over a range of conditions of interest in this work. Initial conditions included an inlet total temperature of 554°K and an inlet static pressure of 1.83 atm. With a mass flow rate of 1.57 kg/sec, the inlet velocity and static temperature were

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159 m/sec and 543°K, respectively; the inlet Mach number was 0.351. Initial turbulent kinetic energy and dissipation rate values were established in the same manner as for the cold flow calculations, and the geometry of the combustor and recirculation zone was the same as in the cold flow calculations.

Both combustion efficiency and wall static pressure distribution data are available for this configuration, and the results of the modular model calculation of these quantities are shown in comparison with the experimental data in Fig. 27. The combustion efficiency was computed from the mass-average temperature at each axial location in the calculation, using the JANNAF temperature-rise combustion efficiency definition. For these data, T_{T5} (ideal) = 2178°K. Note that in these comparisons, data points are shown for the fuel/air ratio 0.053 value at which the computations were carried out. These data points were obtained from plots of combustion efficiency vs. fuel/air ratio presented in Ref. 26 for three different values of combustor L/D. The band shown for each data point represents the range of observed combustion efficiencies as a function of fuel/ air ratio and is a better indication of the overall trend of the combustion efficiency vs. length data than are the individual data points themselves. Some caution is advised in interpreting the combustion efficiency comparison shown in Fig. 27 since three different combustor configurations were involved in obtaining the data. Thus the relationship between recirculation zone length and combustor length is different for each of the three combustors tested....On the other hand, the static pressure data (for the fuel-air ratios which bracket the fuel-air ratio used in the computation) and the predictions are both for a combustor L/D of 3.0.

Overall, the level of agreement with the experimental data is reasonably good, although there is a drop in both combustion efficiency and wall static pressure towards L/D = 3 in the prediction that is not evident in the data. Both of these differences between prediction and experiment may be related to the inaccuracies inherent in the simple one-step global finite-rate model used in these calculations. Of greater interest, however, is the overall low level of combustion efficiency shown by these results, with a maximum combustion efficiency of less than 0.6 at L/D = 3. While this represents a short combustor, the premixed inlet condition should

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alleviate some of the combustion efficiency problems that short, flameholderless sudden-expansion combustors are known to exhibit. In this case the computation shows that the low combustion efficiency arises from the fact that the combustion is premixed. With a uniform directed flow fuel/ air ratio, the recirculation region is also at the same overall fuel/air equivalence ratio which, in this case, is relatively lean ($\phi \approx 0.8$). Thus the recirculation region temperature is lower than it would be at an equivalence ratio nearer 1.0. Since it is the recirculation region that stabilizes the flame, and provides the energy source for flame propagation into the directed flow, this results in relatively slow flame propagation and an overall low combustion efficiency.

While these results indicate a good overall level of agreement with experimental data for a premixed combustor, the nonpremixed case involving liquid fuel injection is of considerably greater practical interest. As a test of the applicability of the modular approach (which, as described in Section 3.4, incorporates a semiempirical model for liquid fuel injection) to the analysis of nonpremixed ramjet combustor flowfield, the experimental configuration tested by Schmotolocha and Economos (Ref. 27) was selected. For these experiments an area ratio $A_2/A_2 = 9$ combustor was used, with liquid JP-4 injected perpendicularly from the inlet walls through an equally-spaced ring of orifices located 6 in. upstream of the dump plane. The inlet air Mach number for this combustor was 0.49 and the global fuel/air equivalence ratio was 0.63. Since the experiments involved a heavy wall combustor, and the code is presently limited to either adiabatic or isothermal wall boundary conditions, the effects of heat loss to the walls on the predicted temperaturerise combustion efficiency were approximated by using a lower air temperature value measured at the exit of the combustor during isothermal testing in place of the actual inlet air temperature.

Model coefficients were taken to be those established from the modeling of the premixed dump combustor described earlier in this section, despite the large difference in dump area ratio between the combustor used by Craig, et al. (Ref. 26) and the present combustor. Results of these compu-

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tations are shown in Fig. 28. In the lower part of Fig. 28, the computed combustion temperature distribution is shown. Coalescence of the isotherms along the recirculation zone boundary reflects the highly turbulent shear layer The predicted equivalence ratio in the recirculation zone, ϕ_{RZ} , is region. 1.87, as compared to a measured value of 1.70, for the globally fuel-lean overall equivalence ratio of $\phi_0 = 0.63$. Note that the vaporization process resulting from liquid fuel injection into the lll0°R airstream effectively reduces the heterogeneous mixture temperature levels, as shown by the presence of a 1000°R isotherm. A comparison of predicted and measured radial temperature profiles is provided at the combustor exit plane. As expected, the measured temperature near the wall is lower than theoretical due to local heat loss. In the region near the centerline the local temperature is substantially underpredicted, which could result from deficiencies inherent in the turbulence modeling or in the global finite-rate chemical kinetics model (which substantially overpredicts the required reaction time compared to a more complete chemical kinetics formulation), or both. However, the mass flow in this region is small relative to the overall combustor mass flow, so that overall combustion efficiency, which is based on mass-averaged temperatures, is well represented. This is shown in the upper part of Fig. 28; the two experimental points represent combustion efficiency obtained from exit species distributions and from exit total temperature.

These results indicate another feature of the modular model, which is its depiction of the details of the flowfield that result from the interaction between the fuel injection process and the distribution of fuel at the inlet and within the recirculation region. For example, a variety of observations have shown that with wall orifice fuel injection, the recirculation zone equivalence ratio is generally more fuel-rich than the overall (global) equivalence ratio. This result has been demonstrated by the data of Schmotolocha and Economos (Ref. 27), which was obtained for three different inlet conditions and at two different locations of the fuel injection orifices upstream of the dump plane. Indeed, the data described in Ref. 27 indicate that for overall equivalence ratios greater than 0.2, the equivalence ratio in the recirculation zone is always greater than

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unity. These data are shown in Fig. 29, in which the results of modular model calculations at two overall equivalence ratios are also shown. The comparison between the data of ref. 27 and the calculations indicates good agreement; what the computational detail shows is that this result arises from the fact that although the peak equivalence ratio in the fuelair distribution at the inlet plane is away from the wall and within the directed flow, the equivalence ratio near the wall and thus adjacent to the recirculation zone downstream of the dump plane is still substantially greater than one.

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Poppet fuel injectors provide, by their design, a fuel penetration that is basically independent of fuel flow rate over their design range. This can be accounted for within the modular model approach by assigning a fixed value for fuel penetration distance and bypassing the fuel penetration calculation described in Section 2.3.4. Fuel mixing and vaporization are still accounted for using the semiempirical approach outlined in the latter section. Recent work carried out at SAI has involved the investigation of ramjet combustor performance characteristics for engines using poppet fuel injectors, for flight conditions representing relatively low Mach numbers. Results of some of this work are shown in Fig. 30; these calculations make use of the version of the modular model incorporating the advanced guasiglobal formulation. The comparison shown in Fig. 30 indicates that the computational results agree very well with the available data. Since a fixed radial fuel injection location was assumed for these calculations, the equivalence ratio in the recirculation region is only slightly above stoichiometric and the temperature is essentially the same in all cases. The performance dropoff observed in both the experimental data and the calculational results as $\phi \rightarrow 1.0$ is a result of the increasing region of fuel-rich equivalence ratio as the overall (global) equivalence ratio approaches one. Combustion in this fuel-rich region results in lower temperatures than are produced by stoichiometric or slightly fuel-lean combustion. Since the ideal equilibrium temperature is that achieved by a one dimensional combustion process starting from the average combustor inlet temperatury and at the average fuel-air ratio of the flow, the actual mass-averaged temperature for the nonuniform stream will remain

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Figure 29. Reciriculation Zone Fuel Concentration



Figure 30. Combustor Performance Prediction, Poppet Injection

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lower, even when all fuel is consumed. Thus there is a dropoff in combustion efficiency that represents the nonuniformity of the flow upstream of fuel ignition in the directed flow.

2.3.7 Discussion

The results documented in this section provide considerable evidence of the overall accuracy of the modular formulation for a ramjet combustor model. They also provide certain insights, particularly with respect to the interaction of the mixing and combustion processes, that are useful in interpreting the results obtained in ramjet test programs. For example, the results just discussed indicate that the high fuel-air ratio efficiency falloff that is often seen in ramjet performance data results from the existence of locally fuel-rich gases when the overall fuel-air ratio is stoichiometric and the fuel is injected just upstream of the combustor inlet. However, the results for a premixed combus? also shown in this section show that at lower overall fuel-air re ; a uniformly mixed inlet stream does not provide high levels of per comance either. In this case, because the inlet flowfield is premixed, and _ an overall low equivalence ratio, the flame-stabilizing recirculation zones are also operating fuel-lean. This results in a recirculation zone temperature that can be considerably less than the stoichiometric flame temperature and thus a reduced rate of propagation of the flame out of the recirculation zones and across the flow. When the fuel is injected from discrete injectors just upstream of the combustor inlet, the modular model results show, in agreement with experiment, that the recirculation zone equivalence ratio is essentially always greater than unity, i.e., fuel-rich. For an overall fuel-lean combustor operation, this results in higher recirculation zone temperatures than would be achieved in a premixed combustor and hence enhanced flame propagation and improved combustion efficiency.

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The value of this approach lies both in its utility as a tool for the investigation of the fundamental mechanisms that inderlie observed ramiet performance trends and in serving as a foundation for further development of more sophisticated approaches, incorporating, for example, treatments of the two-phase flow in a spray combustion situation. Indeed, one of the considerations involved in the development of the spray flame code discussed at the beginning of this section is that it be compatible with and usable as the directed flow portion of a spray-combustor modular model. Combination of this spray code and advanced versions of the boron particle combustion treatments with the modular model framework outlined in this section would provide a useful tool for the investigation of slurry-fuel combustion. Finally, it is possible to incorporate the effects of swirl into the directed flow module while using the stirred-reactor formulation to represent the large-scale recirculation regions that are formed as a result of the application of large amounts of swirl to a flow. Such an extension of the approach would provide a useful tool for the investigation of fundamental phenomena in chemically-reacting swirling flowfields.

2.3.8 Turbulence Models for Ramjet Flowfields

Another aspect of the ramjet modeling work carried out under the present program is the investigation of advanced turbulence models. Although the two-equation $k-\varepsilon$ approach has provided quite widely useful, and is incorporated in the modular model developed as part of this program, it does rest on a gradient diffusion assumption for momentum transfer, and questions have been raised as to the applicability of this approach. The gradient diffusion assumption is avoided if the Reynolds stress equations are solved directly, but this adds three coupled partial differential equations to the set to be solved. If it is assumed, however, that convection and diffusion of turbulence kinetic energy, then the partial differential equations reduce to algebraic expressions and only the turbulent kinetic energy (and turbulent kinetic energy dissipation rate) equations remain to be solved; their solution is accomplished in the same manner as in the two-equation model.

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The assumption that convection and diffusion of Reynolds stress can be related directly to convection and diffusion of turbulent kinetic energy forms the foundation of the algebraic stress model (ASM) first proposed by Rodi (Ref. 28). Since each stress component is obtained directly, this approach avoids use of a gradient diffusion hypothesis. Moreover, for flows in which multiple stress components are apparent, e.g., swirl flows, the ASM approach avoids an isotropic eddy viscosity assumption and avoids any empirical relationship between different stress components. This can result in substantial differences in overall flowfield prediction, as is evidenced by the results shown in Fig. 31. These results are for a constantangle swirl flow at a swirl number of 2, with identical initial and boundary conditions for each computation. Note that while both approaches yield closely similar outer reciriculation zone lengths, there are large differences in the predicted extent and location of the centerline recirculation zones, as well as in the uniformity of the exit flow. This latter characteristic is indicated by the parallelism of the stream function contours at the exit in the k- ε model prediction, compared to the convergence toward the centerline of the stream function contours predicted by the ASM model, as well as the near-wall value of normalized stream function.

Although the results shown in Fig. 31 indicate strong differences between the predictions of the two turbulence model formulations, there is as yet insufficient data with which to evaluate the two approaches, particularly with respect to swirling dump combustor flows. However, work already carried out (Ref. 3) has shown that the use of the ASM formulation does improve predictions in planar recirculating flows with large amounts of streamline curvature, and indirect evidence (such as observations of recirculation zone size and levels of exit-plane nonuniformity) also indicates that further development of the ASM formulation should be pursued.

A second aspect of the comparison of turbulence model results for swirling ramjet combustor flowfields involves the examination of the effects of different initial swirl distributions. An example of this is provided by the results shown on Figs. 32 and 33, which show radial profiles of axial (Fig. 32) and tangential (Fig. 33) velocity, for a swirling flow in a 1.5:1

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diameter ratio sudden expansion for four different types of inlet swirl. Note that the low area ratio was chosen to minimize inertial effects and thus maximize the effects of the turbulence model formulation on the flowfield prediction. The overall swirl number in this demonstration is held constant at 0.4, and there is a centerbody at the origin of this flow (within the inlet). A nonuniform 37 (axial) by 26 (radial) grid was used, and predictions are shown for both a two-equation and ASM turbulence model. Despite the small size of the figures, it is immediately apparent from the tangential velocity profiles shown in Fig. 33 that the ASM approach prediction of the downstream mixing-out process differs substantially from that predicted using the two-equation approach. It was noted earlier that there is a tendency in the work reported in the literature for predictions of swirl flows to relax to a profile characteristic of a forced vortex, war, whatever the initial tangential velocity distribution. Such a tendency is observable in the profiles predicted using the k- ε approach shown on Fig. 33(a), but the ASM predictions, Fig. 33(b) do not exhibit this tendency. This effect thus appears to be directly related to the existence of an isotropic eddy viscosity assumption implicitly in the k- ϵ model application, whereas with the ASM (different) effective viscosities are obtained for each of the three shear stress components.

2.4 MODELING OF THE DUCTED ROCKET COMBUSTION PROCESS

The work being carried out in this program under the task area outlined in Section 1(d) had as its objective the development of a new theoretical model to describe the three-dimensional reacting flow typical of multiple-inlet ducted-rocket combustion chambers. It was supported, through AFOSR, by the Ramjet Division (RJT), AFWAL. Because of the paucity of experimental data on the aerodynamics of the ducted rocket configuration, the modular model development work under this task area utilized the hierarchy of models concept, in which unified elliptic aerodynamic models were used to define characteristic flowfield regions for the development of modular models which incorporate the fundamental chemical kinetic formulations required to address the performance aspects of ducted rockets.

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Aerodynamic calculations were carried out for a three-dimensional configuration similar to an experimental ducted rocket combustor tested at AFWAL/RJT. The three-dimensional elliptic analysis used for these computations was a modified version of an analysis similar to the Imperial College TEACH code, incorporating a two-equation turbulent kinetic energy turbulence model similar to that used for the computations described in Sections 2.1 and 2.3. A three-dimensional grid is, of course, required, with 21 axial, 10 radial, and 18 circumferential grid points. This grid is not fine enough to provide grid-independent results, but since it involves 3780 node points it is a compromise between the fineness needed to obtain grid-independence and the limitations of computer storage and speed*. The configuration examined involves two symmetrically-disposed inlets at 180° apart: this is not identical to the AFWAL configuration but was selected to simplify the implementation of boundary conditions in these computations. A sketch of this combustor geometry is shown in Figure 34, from which it can further be seen that the inlets are disposed at an angle of 45° to the longitudinal axis of the combustor. The air inlet velocity was selected to correspond to an airflow rate of 2 lb/sec/inlet.

The velocity vectors computed for this flow field in a plane through the inlets and along the combustion centerline are shown in Fig. 35. Two recirculation zones can be seen, one at the head end of the combustor and the second along the outer walls just downstream of the inlets. Contours outlining the approximate sizes of these recirculation regions are shown on Fig. 35. For fuel injection in the inlet arms (i.e., the side-dump liquid fueled ramjet configuration) both of these recirculation regions are potential flameholding sites. However, if fuel is injected from the combustor head end (the ducted rocket configuration) it would be expected that the primary flameholding region would involve the recirculation zone at the combustor head end.

^{*}The solution procedure involves eight variables: three velocity components, the pressure, the flow enthalpy, and a species used as a tracer, as well as the turbulent kinetic energy and its dissipation rate. Thus for the grid noted, 30,240 locations are required for the storage of the dependent variables alone, for this nonreacting (but possibly nonisothermal) calculation.











The radial extent of the recirculation zone at the head end of the ducted rocket combustor is depicted in Fig. 36. Of interest in this view are the distinctive four-lobed shape of the recirculation region and the stagnation point shown on the flowfield centerline. Through computations such as represented by Figs. 35 and 36 it is possible to build up a three-dimensional view of the size and shape of the recirculation zones in the ducted rocket combustor. This provides one of the required pieces of information for the development of a modular model of this flowflield.

Various types of modular models can be postulated for a flowfield such as shown in Figs. 35 and 36. However, one of the most useful, because of its computational speed and flexibility, is the well-stirred reactor/plug flow with distributed secondary injection/entrainment approach. In this model the intense mixing that occurs in the region of the inlets in the ducted rocket combustor is modeled using a well-stirred reactor formalism, while the subsequent mixing and combustion of fuel and air not transported into the recirculation zone is modeled as a plug flow with distributed entrainment. While this approach is fast and flexible, it requires, in addition to a specification of the size and shape of the recirculation zone, a measure of the proportion of the flow involved in the recirculation region and in the subsequent mixing region. This specification of the proportion of the flow found in different regions can be provided using the elliptic aerodynamic formulation with a species tracer.

Calculations carried out to date to examine the mixing and kinetics limitations within the side-dump combustor used at AFWAL have not been successful. In part this state of affairs arises from the complexity of the overall flowfield, but in general the characteristics of the combustor appear to be such that kinetics are not limiting. Mixing-limited situations are inherently more difficult to approach with the sort of modular model being applied in this phase of the program. The work in this specific area is continuing under a follow-on AFOSR contract.

It should be noted that the configuration tested at AFWAL is not a true ducted rocket but represents a side-dump ramjet combustor configuration. One of the essential features of a ducted rocket is the presence at the head end of the combustor of one or more jets of higher temperature,

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fuel-rich, partially reacted products of the rocket combustion process. These jets are sonic, or more usually, highly underexpanded supersonic flows. Thus the flowfield within a true ducted rocket involves both subsonic and supersonic regions, with strong shock and pressure wave interactions, and could be expected to be considerably different in character from the flowfield shown in Figs. 35 and 36. This aspect has not been accounted for in any ducted rocket modeling so far described and will be considered in continuing SAI work in this area.

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3. PUBLICATIONS

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- 6. Harsha, P.T., and Edelman, R.B., "Computational Hierarchy for the Analysis of Combustion Phenomena in Ramjet Environments" Presented at 1984 JANNAF Propulsion Meeting, New Orleans, 7-9 February 1984. To be published by CPIA.
- 7. Harsha, P.T., and Edelman, R.B., "Analytical Modeling of a Spray Diffusion Flame," AIAA Paper 84-1317, Presented at AIAA/SAE/ASME 20th Joint Propulsion Conference, Cincinnati, 11-13 June 1984. Submitted for publication in AIAA Journal.

4. PROFESSIONAL PERSONNEL

The following personnel have contributed to the work discussed in this report:

- 1. Dr. R.B. Edelman
- 2. Dr. P.T. Harsha
- 3. Dr. T.-S. Wang
- 4. Dr. M.M. Sindir
- 5. Mr. W.N. Bragg
- 6. Mr. G.C. Cooper
- 7. Mr. C. Morrison

5. INTERACTIONS

5.1 PRESENTATIONS

During the course of this work, the following presentations were made:

- 1. "Combustion Modeling for Practical Applications," Presented at ASME Fluids Engineering Conference, June 22-24, 1981.
- "Interpretation of Ramjet Combustor Test Data," Presented at AIAA/ SAE/ASME 17th Joint Propulsion Specialist' Conference, July 22-29, 1981.
- 3. "Combustion Modeling for Ramjet Development Programs," Presented at AGARD Propulsion and Energetics Panel 58th Symposium, October 26-29, 1981.
- 4. "Mixing, Ignition and Combustion in Flowing, Reacting Fuel-Air Mixtures," Presented at 1981 AFOSR Combustion Dynamics Contractors' Meeting, Nov. 16-20, 1982.
- 5. "Mixing, Ignition and Combustion in Flowing, Reacting Fuel-Air Mixtures," Presented at 1982 AFOSR Combustion Dynamics Contractors' Meeting, Nov. 1-4, 1982.
- 6. "Modeling of Multi-Phase Flows in Ramjet Combustors," Presented at 1983 JANNAF Propulsion Meeting, Monterey, CA, February 15, 1983.
- 7. "Fundamental Processes in Spray Combustion" Presented at 1983 AFOSR Combustion Dynamics Contractors' Meeting, Sept. 19-23, 1983.
- 8. "Kinetics Limitations in the Consumption of Particulate Boron," Presented at 1983 AFOSR Combustion Dynamics Contractors' Meeting, Sept. 19-23, 1983.
- 9. "An Approach to Non-Gradient Diffusion in the Analysis of Turbulent Combustion" Presented at 1983 AFOSR Combustion Dynamics Contractors' Meeting, Sept. 19-23, 1983.
- "Computational Hierarchy for the Analysis of Combustion Phenomena in Ramjet Environments" Presented at 1984 JANNAF Propulsion Meeting, New Orleans, February 7-9, 1984.
- 11. "Analytical Modeling of a Spray Diffusion Flame" Presented at AIAA/SAE/ ASME 20th Joint Propulsion Specialist' Conference, June 11-13, 1984.
- 12. "Ducted Rocket Combustion Modeling" Presented at JANNAF Workshop on Ducted Rocket Combustors, Cincinnati, OH, June 13, 1984.
- 5.2 CONSULTATIVE AND ADVISORY FUNCTIONS

Two of the task areas of this program involve continuing and formal

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interactions with DOD laboratories. The ducted rocket modeling work carried out under the task area outlined in Section 1(d) involves close interaction with experimental work carried out by Drs.'F.D. Stull and R.D. Craig at AFWAL/ RJT. In addition, the boron slurry modeling effort described in Section 1(c) involves coordination with experimental work being done by Dr. Klaus Schadow at NWC.

In addition, Dr. Edelman served on the Propuslion Technology Panel of the Military Space System Technology Model (MSSTM) evaluation activity for the Space Division of the Air Force Systems Command, and Drs. Edelman and Harsha have both been active in participating in JANNAF-sponsored workshops on swirl flows in ramjets, two-phase flow in ramjet combustors, and ducted rocket combustion technology.

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