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CHEMICAL KINETIC/GAS DYNAMIC/PARTICLE INTERACTIONS IN ROCKET NOZZLE AND EXHAUST PLUME FLOWS

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I. INTRODUCTION

This research program has been directed towards obtaining a fundamental understanding of chemical kinetic/gas dynamic/particle interactions in rocket nozzle and exhaust plume flows. The work is motivated primarily by the need for accurate predictions of such rocket plume observables as IR radiation, radar cross-section and visible smoke. The nozzle flow studies have emphasized the determination of gas and particle properties at the exit plane which are used as input to rocket plume codes; the plume work has primarily concentrated on determining IR radiation properties of low altitude afterburning plumes from subscale liquid propellant motors. An additional effort has been directed toward the calculation of particle flows in afterburning plumes with the ultimate goal of predicting the visibility of low signature propellant plumes.

II. ACCOMPLISHMENTS

A. Fully-Coupled Rocket Nozzle Flow Model/Computer Code

A significant advance in nozzle flow calculations was achieved with the development, under this contract, of a fully-coupled rocket nozzle flow model and computer code (FULLNOZ).[1] The model simultaneously treats chemical kinetics and particle/gas thermal and dynamic nonequilibrium effects for contoured nozzles, including the influence of the wall boundary layer. The computer code is based on the MULTITUBE code developed by Boynton,[2] which utilizes the streamtube method (as described by Boynton and Thomson[3]) to integrate the hyperbolic governing equations of steady supersonic flow. Basically, this method solves the corresponding finite-difference equations along and perpendicular to streamlines. The elliptic Navier-Stokes equations are reduced to hyperbolic form by assuming that diffusional effects along streamlines are small compared to diffusion across streamlines. This is a very good assumption for nozzle flows and enables one to solve an initial value problem (where a marching procedure can be used), rather than the more difficult boundary value problem.

The operation of FULLNOZ is relatively straightforward, starting with the specification of initial gas and particle properties just downstream of the throat (Mach number > 1) and the nozzle wall contour. Additional input data

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1. Pergament, H.S. and Thorpe, R.D., "A Computer Code for Fully-Coupled Rocket Nozzle Flows (FULLNOZ)," AeroChem TP-322, AFOSR TR-75-1563, April 1975.

2. Boynton, F.P., "The MULTITUBE Supersonic Flow Computer Code," General Dynamics/Convair GDC-DBB 67-003, February 1967.

3. Boynton, F.P. and Thomson, A., "Numerical Computation of Steady, Supersonic, Two-Dimensional Gas Flow in Natural Coordinates," J. Computational Phys. 3, 379-398 (1969).

include the thermodynamic properties of all constituent chemical species (which are incorporated via curve fits of JANNAF data), a chemical reaction mechanism and rate coefficients, the physical properties of the particles and the nozzle wall temperature (for the boundary layer calculations). The marching scheme proceeds downstream, from one orthogonal (to the flow streamline) surface to the next, computing flow properties and composition within a specified number of streamtubes. At each orthogonal surface the code also calculates wall shear stress and heat transfer, boundary layer displacement thickness and velocity and temperature profiles, coupling the shear stress and heat transfer to the 'wall' streamtube properties. The turbulent boundary layer analysis utilizes the Van Driest transformations[4] and the experimental data of Keener and Hopkins,[5] which relate the compressible skin friction coefficient to measured velocity/temperature profiles in flows with favorable pressure gradients. Coupling between the boundary layer and 'wall' streamtube properties is achieved via solution of the momentum integral equation to give boundary layer momentum thickness as a function of distance along the nozzle wall. The displacement thickness is then determined from the velocity profile and the momentum thickness.

FULLNOZ has now been established as an operational code for analyzing rocket nozzle flows. It has been delivered to the Air Force Rocket Propulsion Laboratory (AFRPL) and, via AFRPL, is available throughout the country to industrial and government laboratories. It will be used by Lockheed/Palo Alto as part of their visible plume signature study for AFRPL. AeroChem has used it extensively for AFRPL (under subcontract to Aerodyne Research, Inc.) to predict nozzle exit plane properties for a number of solid and liquid propellant tactical and strategic missiles. These properties were then used by AeroChem as input to the calculation of exhaust plume electrical properties (electron density and electron-neutral collision frequency) which in turn were input to plume radar cross section calculations made by Aerodyne. In addition we have used FULLNOZ to calculate gas and particle properties within the Space Shuttle solid rocket booster nozzle.[6]

The speed and versatility of FULLNOZ are demonstrated in Table I, which summarizes input conditions and computer run times for several types of systems of interest to the Air Force. The usefulness of FULLNOZ can be further

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4. Van Driest, E.R., "Turbulent Boundary Layer in Compressible Fluids," J. Aeron. Sci. 18, 145-160 (1951).

5. Keener, E.R. and Hopkins, E.J., "Van Driest Generalization Applied to Turbulent Skin Friction and Velocity Profiles Measured on the Wall of a Mach 7.4 Wind Tunnel," AIAA J. 11, 1784-1785 (1973).

6. Pergament, H.S., Thorpe, R.D., and Hwang, B., "NO_x Deposited in the Stratosphere by the Space Shuttle Solid Rocket Motors," Final Summary Report, Phase II, AeroChem TP-333, NASA CR-144928, December 1975; see also, Thorpe, R.D., Pergament, H.S. and Hwang, B., "NO_x Deposition in the Stratosphere by the Space Shuttle Solid Rocket Motors," JANNAF 9th Plume Technology Meeting, CPIA Publ. 277 (Applied Physics Lab., Johns Hopkins Univ., Silver Spring, April 1976), pp. 317-352.

TABLE I

DATA ON FULLNOZ RUNS

	No. of Gas Species	No. of Chemical Reactions	No. of Particle Groups	Chamber Pressure, atm	Nozzle Throat Radius, cm	Nozzle Area Ratio	Nozzle Length, cm	Computer Run Time, sec		
								CDC[a] 6400	CDC[b] 6600	CDC[b] 7600
Liquid (MMH/N_2O_4)	17	20	0	170	14.6	60	220	186	50	7
Liquid (MMH/N_2O_4)	17	20	0	170	7.66	60	116	187	50	7
Solid (16% Al)	16	19	4	119	2.3	7	22.5	356	90	13
Solid (16% Al)	16	19	4	36	2.98	7.14	40	160	40	6
Solid (19% Al)	16	19	4	44.2	5.96	7.78	50.6	193	50	7

[a] Actual run time on AFRPL CDC 6400.

[b] Estimated.

enhanced by the incorporation of a transonic flow solution (e.g., that of Nickerson and Kliegel[7]) to allow the code to start at the combustion chamber rather than downstream of the throat. Other modifications that can easily be made which would extend the capability of FULLNOZ include: (1) low Reynolds number flows, where the boundary layer is a large portion of the nozzle flow, (2) nozzle film cooling, i.e., the effects of mass injection on wall heat transfer and shear stress, and (3) nozzle-induced shocks.

B. Interpretation of IR Radiation Data on Subscale Liquid Propellant Motor Plumes

Data obtained by the Air Force Armament Laboratory[8] on subscale kerosene/oxygen rocket motors (fired into a vacuum tank) have shown that measured IR plume radiation in the 4-5.5μ band is in sharp disagreement with predictions using state-of-the-art modeling techniques. These techniques include: (1) thermochemical equilibrium chamber and nozzle calculations, (2) a coaxial turbulent mixing/nonequilibrium chemistry exhaust plume analysis and (3) IR radiation 'band model' calculations with CO_2 as the radiating species. The

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7. Nickerson, G.R. and Kliegel, J.R., "Axisymmetric Two-Phase Perfect Gas Performance Program," TRW Systems Report No. 02874-6006-R000, Vols. I and II, April 1967.

8. Ebeoglu, D.B. and Martin, C.W., "Experimental Verification of Infrared Plume Predictions for a Rocket Engine," AFATL-TR-74-191, November 1974; see also, Ebeoglu, D.B., Martin, C.W., Breil, S., Victor, A., Mantz, J., and Rothschild, W.J., AIAA Paper No. 75-1231; AIAA/SAE 11th Propulsion Conference, Anaheim, California, 29 Sept. - 1 Oct. 1975.

nature of the discrepancy between measured and predicted radiation is that for O/F ratios less than stoichiometric the total radiant intensity is much greater than that predicted by the model, while for high O/F ratios the model overpredicts the data. The goal of our work under this contract was to explain the discrepancies between theory and experiment and to develop a model which can reliably be used to predict the plume gas dynamic and chemical properties.

A careful evaluation of all assumptions utilized in the original predictions demonstrated that the most probable cause for the failure of the model is that it did not account for the effects of the (observed) incomplete combustion in the rocket motor chamber. Based on this observation a new 'phenomenological' model was developed which assumes that some of the fuel does not burn in the chamber but is pyrolyzed to a lower order hydrocarbon before leaving the rocket nozzle. The amount of fuel unburned is then determined by comparing the measured rocket performance (the C* efficiency) to that predicted via thermochemical equilibrium calculations. This determination is made by assuming: (1) a fixed percentage of the fuel does not burn but forms a specific pyrolysis product (e.g., C_8H_{16}, C_2H_4 or CH_4, etc.) from the liquid kerosene and (2) the pyrolysis product remains inert in the chamber and nozzle expansion. The percentage of unburned fuel leaving the nozzle is assumed to be that amount for which the measured and calculated C* efficiencies are equal. The model further assumes that, upon entering the plume, the unburned fuel participates in three overall kinetic processes: gas phase oxidation, polymerization to form soot and soot oxidation. These global processes are coupled to the conventional ten-step CO/H_2 oxidation scheme through the following three reactions.

Gas-phase Oxidation:

$$(CH_2) + OH \rightarrow CO + H_2 + H$$

Soot Formation:

$$n(CH_2) \rightarrow (CH_2)_n$$

Soot Oxidation:

$$(CH_2)_n + nO_2 \rightarrow nCO + nH_2O$$

where (CH_2) represents an arbitrary fuel fragment.

The results obtained to date[9] (shown in Fig. 1) have incorporated only the gas-phase oxidation step. For $O/F = 1.8$ ($(O/F)_{stoich} = 3.5$) the results indicate that accounting for the effects of unburned fuel via the above model will give substantially increased plume temperatures and IR radiation if the turbulent mixing rate (ambient air with exhaust products) is such that all

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9. Pergament, H.S., Thorpe, R.D., and Miller, W.J., "Interpretation of IR Radiation Plume Data on Subscale Kerosene/O_2 Rocket Motors," JANNAF 9th Plume Technology Meeting, CPIA Publ. 277 (Applied Physics Lab., Johns Hopkins Univ., Silver Spring, April 1976), pp. 125-143.

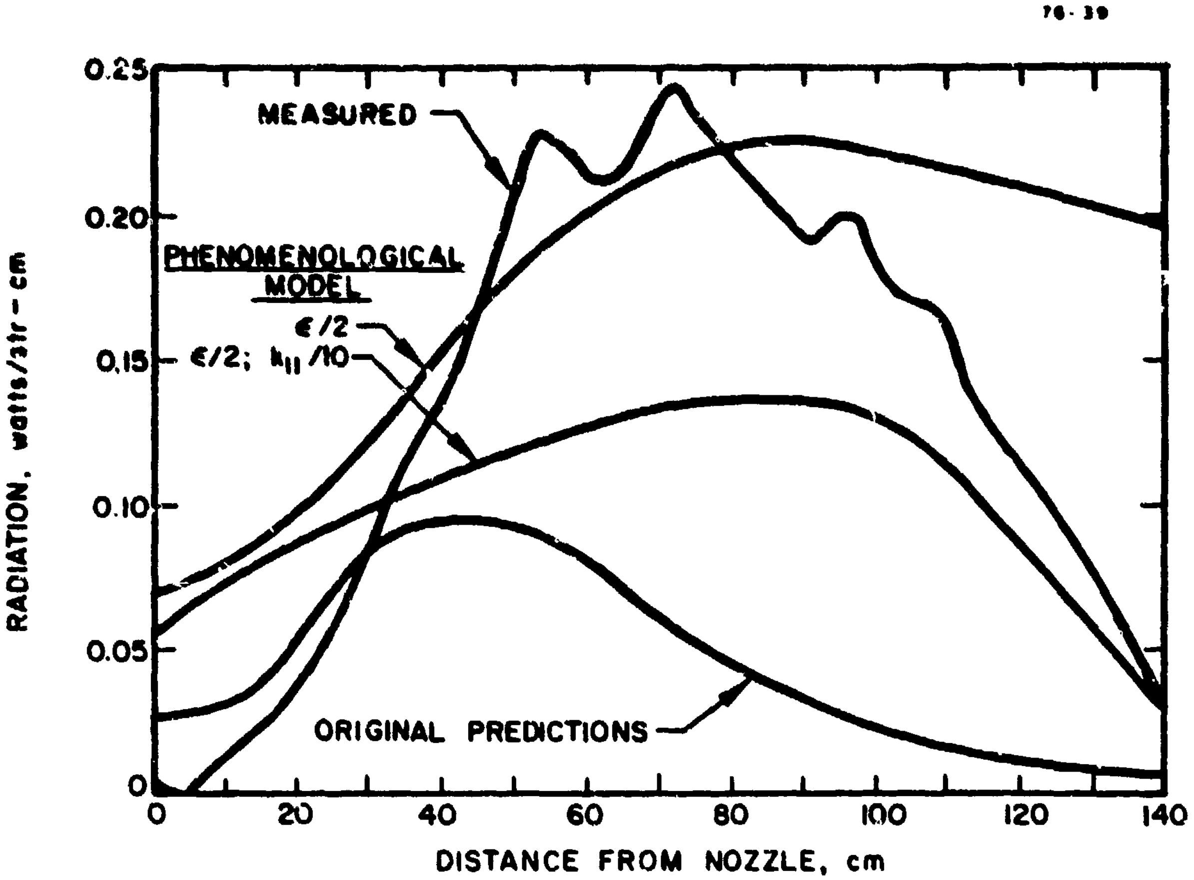

Fig. 1 Comparison between measured station radiation (O/F = 1.3) and predictions with phenomenological model.

Original predictions from Ref. 8; ε = eddy viscosity coefficient; $(CH_2) + OH \xrightarrow{k_{11}} CO + H_2 + H$; $k_{11} = 1 \times 10^{-11} \exp(-7000/RT)$; (CH_2) is unburned fuel.

the 'unburned fuel' burns in the plume. This increased level of IR radiation is in much better agreement with the IR data than the original predictions, demonstrating the general validity of the new phenomenological model.

Much work remains to be done before the new model can be generally accepted as a viable calculational procedure for this type of afterburning plume. This work should include:

(1) Comparisons between predictions and data over the entire range of O/F for which radiation measurements were made.

(2) Establishing an eddy viscosity coefficient consistent with the actual plume velocity field.

(3) Determining the influence of inaccuracies in measured C^*_{eff} on the predictions, via a series of parametric calculations in which the % un burned fuel is varied over a reasonable range.

(4) Incorporating the soot formation and oxidation steps in the afterburning plume reaction mechanism.

(5) Comparisons between theory and experiment for the more recent set of data obtained at AFATL.[10,†] These data were taken on the same motors, but with mass flows of 5 g/sec (in contrast to 9 g/sec for the test data interpreted in the present work) and burned benzene (C_6H_6) and methane (CH_4), in addition to kerosene.

Because unburned hydrocarbons entering the plume are apparently primarily responsible for the large IR signatures of these plumes for rich mixtures, the following practical conclusion can be drawn: The 'rocket motor' used for the simulation studies should be designed a priori as a hydrocarbon fuel injector, with (possibly) direct injection into the plume rather than with unburned fuel injected as a result of incomplete combustion in the chamber.

C. Particle Motion in Afterburning Rocket Plumes

The purpose of this task was to develop a computational tool to describe particle motion in afterburning rocket plumes. Specifically, we have incorporated the particle subroutine in FULLNOZ (subroutine DRAG), which numerically evaluates the gas/particle interaction terms, into the AeroChem Low Altitude Plume Program[11] (LAPP), the standard tool throughout the country for computing afterburning plume properties. The gas phase momentum and energy equations in LAPP have been modified to account for these interaction terms and the particle conservation equations have been formulated in streamline coordinates for use in Lapp. These equations must be coded and the LAPP input format modified to accept particle data in order to develop an operational code. Once these tasks have been completed, the LAPP code will be able to accept input data on nozzle exit plane gas and particle properties and routinely compute gas and particle temperatures and velocities in afterburning plumes.

[†] These comparisons are being made as part of the Cooperative Plume Modeling Program under the auspices of the TTCP W-4 panel. Further information may be obtained from Capt. W.J. Rothschild, DLMQ, Air Force Armament Laboratory, Eglin AFB, FL.

10. Rothschild, W.J. and Martin, C.W., "Experimental Results for Hydrocarbon Exhaust Infrared Model Verification," AFATL-TR-76-74, July 1976.

11. Mikatarian, R.R., Kau, C.J., and Pergament, H.S., "A Fast Computer Program for Nonequilibrium Rocket Plume Predictions," Final Report, AeroChem TP-282, AFRPL-TR-72-94, NTIS AD 751 984, August 1972.

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A review of the accomplishments achieved under this AFOSR contract is presented. Among the most notable are: (1) the development and demonstration of a fully-coupled rocket nozzle code (FULLNOZ) which, in calculating nozzle flow properties, couples the effects of nonequilibrium chemistry, gas/particle thermal and dynamic nonequilibrium, turbulent mixing across streamtubes and turbulent wall boundary layers and (2) the development of a phenomeno-logical model for the interpretation of IR radiation data from subscale liquid propellant rocket motor plumes; the model accounts for the effects of unburned fuel on rocket nozzle and afterburning plume properties.

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