Chemical Modeling Experimental Facility

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A high-temperature turbulent jet facility has been constructed for the purpose of partially simulating a turbulent, chemically reacting, hypersonic wake. A mass spectrometer which is movable throughout the jet allows detailed studies of the evolution of the chemistry, particularly the ionic species, produced via the interaction of high-temperature air and ablation products with subsequently entrained cool ambient air. Measurements have been performed in this facility on N_2/O_2 mixtures, and axial and radial species concentrations of air ions have been obtained.

I. Introduction

A NEW facility, the Chemical Modeling Experimental Facility (CMEF), has been constructed to aid in the understanding of the chemistry in a high-temperature turbulent wake. In this facility, a high temperature turbulent jet is produced that partially simulates a turbulent, chemically reacting, hypersonic wake. The evolution of the jet chemistry (particularly the ionic species) produced via the interaction of the high temperature air and ablation products with subsequently entrained cool ambient air is studied with a movable quadrupole mass spectrometer.

II. Experimental Facility

A schematic diagram of the facility is shown in Fig. 1a. A 50 kw rf induction arc§ is used to heat air (or other combinations of gases) to chemically simulate near wake conditions. Typically, the arc is maintained in an 80% N_2-20% O_2 flow of 1 g/sec at a pressure of a third of an atmosphere. The hot gas is expanded into a mixing chamber where other species, such as ablation products, may be added, and the mixture is expanded as a free subsonic turbulent jet into a partially evacuated chamber containing air. As the jet flows downstream, it entrains and reacts with the ambient air in a manner similar to that of a turbulent wake. In both cases, a hot stream mixes turbulently with a cooler one causing temperature changes and chemical reactions. The correspondence with a wake is not direct since the entrainment occurs in a much shorter distance causing a correspondingly more rapid decrease in the jet temperature and velocity. The larger rate of entrainment of the surrounding air by the jet also causes the time a particle spends in the jet to increase as the square of the distance, whereas the time a corresponding particle spends in a wake increases only linearly. The net effect is to simulate closely the time history of wake temperature and species concentration. The more rapid entrainment of the jet makes the laboratory experiment feasible, since for a given initial size and wake length of interest, the jet reaches the flow conditions corresponding to this wake length in a relatively short distance. Thus, the jet cools from a few thousand degrees at the exit nozzle to ambient temperatures in a few meters.

In order to have direct chemical scaling between the jet and wake at the altitudes of interest, the ambient pressures are matched. The chemical processes in the jet and wake are then the same and chemical scaling is not necessary. This is important in cases for which the proper scaling law is uncertain because of simultaneous unimolecular, bimolecular, and termolecular reactions.

A large apparatus was required for the facility in order to allow operation at low pressures with a turbulent jet. To provide the mass entrained by the jet flow, gas injection rings line the periphery of the tank (Fig. 1a). These injection rings and the pumping at the end of the tank allow the establishment of a

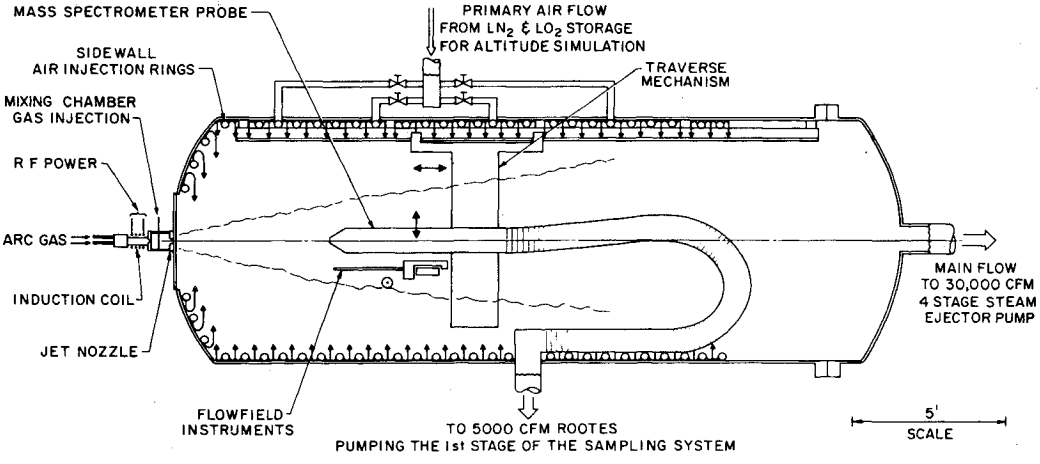

Fig. 1a The chemical modeling experimental facility—schematic.

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§ Lepel 50 kw rf supply with a Tafa, Induction Plasma Torch.

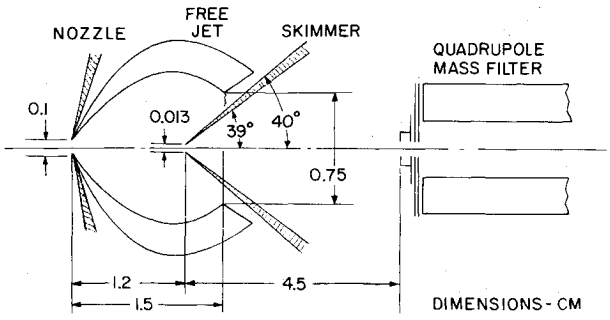

Fig. 1b The CMEF sampling geometry—schematic.

flow approximately that of a jet into an unbounded medium at rest.

The gas supply and the vacuum chamber have been assembled with special care for cleanliness. The desired gas impurity level is less than 10 ppm. Liquefied nitrogen and oxygen are purchased in bulk with a guaranteed impurity analysis better than 10 ppm. The liquid gases are vaporized, metered, mixed, and piped to the experiment in carefully cleaned apparatus and piping.

A major capability of this facility is the in situ measurement of species concentrations in the high temperature, chemically reacting, turbulent jet using a movable quadrupole mass spectrometer. Since the spectrometer requires a low background pressure for proper operation (typically less than 10^{-5} torr), a special flow sampling system was designed to match this pressure to the jet pressure (typically tens of torr) and at the same time minimize any distortions of the high temperature chemical composition due to the sampling process. The design is an extension of the concept originally proposed by Kantrowitz and Grey[1] and is shown schematically in Fig. 1b.

Basically, the gas from the high temperature turbulent stream is extracted through a small ($\sim$1-mm-diam) nozzle as an underexpanded, supersonic, axisymmetric free jet. This flow causes the gas sample to cool rapidly, freezing its chemical composition. A small axial portion of the freejet is then passed through a truncated conical molybdenum skimmer having an orifice at its apex. A molecular beam is thereby produced and mass filtered using a quadrupole spectrometer. A 2-in. diffusion pump is used to maintain a vacuum of nominally 10^{-5} torr in the quadrupole section.

The diameter of the nozzle which forms the freejet was determined so that it satisfied two criteria. The first was that the sample which is withdrawn through the nozzle orifice should not be from the boundary layer which forms on the outer surface of the nozzle as the turbulent flow moves past. A calculation was made to make this criterion quantitative by considering the orifice as a sink at the stagnation point of the boundary-layer flow. This resulted in the requirement that the Reynolds number based on the sonic conditions in the orifice and the orifice diameter be greater than approximately twenty. The second was that the diameter of the nozzle be small enough so that the pumping in the region between the nozzle and the skimmer could be adequate to produce a freejet of large enough dimensions so that the insertion of the skimmer cone through the Mach disk would not interfere with the intercepting shock. This was verified for the 1-mm nozzle using the measured pressure ratios obtained with a 5000-cfm Rootes blower and the results presented in Refs. 2 and 3.

The location and cone angle of the skimmer were chosen to conform to the results of previous molecular beam studies.[4-6] The location is ahead of the freejet Mach disk at a point where the density is computed to have fallen by a factor of approximately 800 from its value at the nozzle. The computed mean free path here is roughly 60 times the diameter of the skimmer orifice shown, while the Mach number is about 12. This makes the local Knudsen number (based on skimmer orifice diameter) to Mach number ratio about 5, for which value the cited references indicate the best sensitivity and broadest response (i.e., best molecular beam) over the pressure and temperature ranges of the turbulent flows to be sampled. In the position shown, the skimmer is advanced slightly upstream of the point where it is estimated that background gas can reach the freejet axis and influence the species concentrations.[4] The external skimmer cone angle was made as large as possible consistent with maintaining an attached shock downstream of the leading edge to prevent entrance interference. The leading edge was machined to be as sharp as possible (approximately 0.025 mm) and still maintain sufficient structural strength to prevent feathering. With the large external angle, the internal angle could be made correspondingly large to maintain high particle conductance downstream of the skimmer and into the quadrupole filter. This filter has a standard ionizer/lens system and an extended range of from 0 to 650 amu with typical resolution, $m/\Delta m$, of 150. Before operation, the entire sampling system is very carefully aligned using a laser beam as reference.

A traversing mechanism was constructed for the mass spectrometer and the flowfield instruments in order to allow mapping of the chemical evolution in the jet. Axial and vertical motion was provided for the mass spectrometer over 14 ft of the length of the tank and 4 ft vertically. An 8-in. stainless-steel flexible tube was used to provide the pumping required for the first stage of the sampling system. The flowfield instruments also are movable 4 ft horizontally transverse to the jet axis. The mass spectrometer is capable of measuring either positive, negative or neutral species. Ionic concentrations as low as 10^{-12} of the total jet density have been measured, while neutral concentrations of 10^{-5} can be determined. Other diagnostics include temperature probes, an electrostatic probe for electron concentration measurement, a hot wire anemometer for measuring velocity profiles and a calorimeter for measuring the total enthalpy in the jet.

III. Measurements

Jet Growth

The thermal characteristics of the jet were measured using a shielded thermocouple mounted on the traversing probe table. The experimental results for one set of arc and exhaust tank conditions are presented in Figs. 2a and 2b. In Fig. 2a, the experimental point at the exhaust plane was obtained using a calorimetric heat balance to measure the enthalpy flux and an equilibrium chemistry program to calculate the corresponding temperature. The axial temperature data are fit with a curve of the form $1+A/(X-X_0)$, where $A=100$ and $X_0=3$ cm when $X-X_0$ is expressed in cm. This behavior is similar to that of

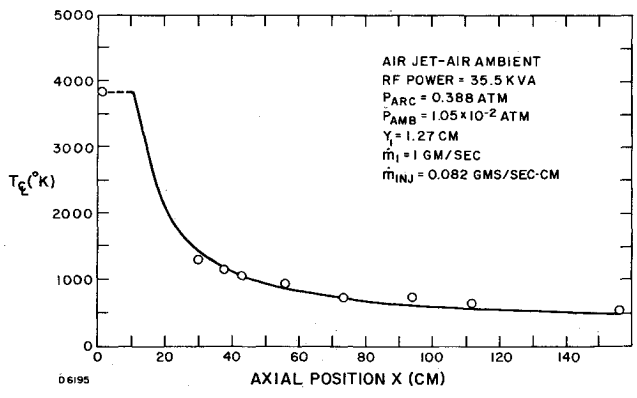

Fig. 2a Axial temperature profile. Data are fit with a $T=3\times10^2+3\times10^4/(X-3)$ dependence. P_{ARC} is the arc stagnation pressure, P_{AMB} is the ambient pressure, Y_1, $\dot{m}_1$ are the initial jet radius and mass flow, $\dot{m}_{INJ}$ is the peripheral mass injection rate.

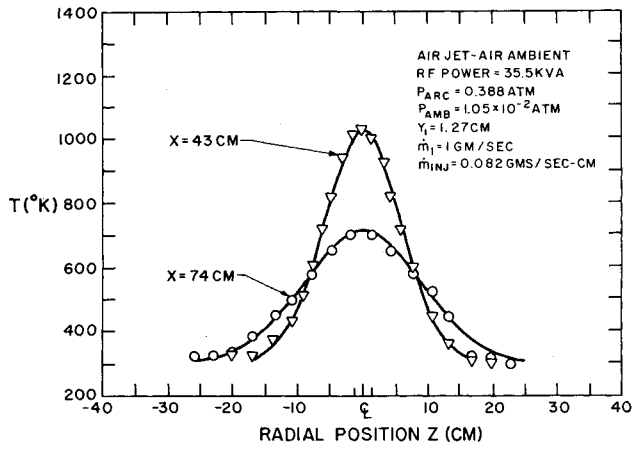

Fig. 2b Radial temperature profiles—horizontal. Data are fit with gaussian curves.

the data assembled by Laufer[7] and that obtained by Demetriades and Doughman.[8] The radial temperature data are accurately fit with Gaussian profiles. Again, this is in keeping with the assumption of Laufer[7] and the findings of Demetriades and Doughman[8] and O'Conner, Comfort and Cass,[9] and indicates that the jet is indeed self-preserving.

Ion Measurements

The first experiments have been performed on studies of the clean air negative ion cycle with the initial measurements being obtained downstream in the cooler regions of the jet. A set of axial profiles for several of the air negative ions is shown in Fig. 3a. They appear at distances greater than about 120 cm as the electrons in the flow begin to attach. Following the NO_3^- profile (NO_3^- being the terminal negative ion in the air kinetic model[10]), it appears that by 160 cm the NO_3^- concentration peaks due to the electrons being fully attached, and thereafter, decays due to dilution by ambient gas entrained by

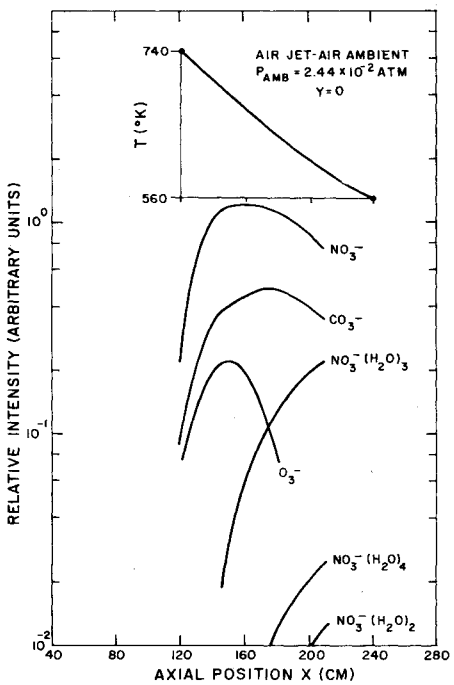

Fig. 3a Axial species concentration profiles.

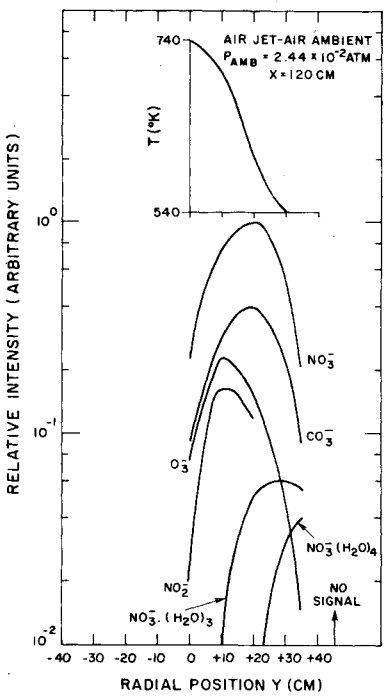

Fig. 3b Radial species concentration profiles—vertical.

the jet. Also, in these cooler regions of the jet, the hydrates of NO_3^- can be seen to form due to a small amount of residual water vapor in the tank.

Figure 3b shows radial profiles of the jet taken at an axial distance of 120 cm from the exhaust plane. The jet temperature is seen to be maximum on the centerline. Again, as lower temperatures are approached at the jet boundary, the negative ion concentrations are seen to increase and then fall. By a radius of 45 cm, no charged species are present in fractional concentrations greater than the system sensitivity of about 10^{-12}.

Concentrations in the hotter regions of the jet are presently being measured. In these regions, the presence of NO^+, O^-, O_2^-, O_3^-, NO_2^- and NO_3^- is observed in general support of the predictions of the kinetic model of Sutton.[10]

IV. Conclusions

The important capability of the CME is its ability to study the chemistry of complicated systems occurring in turbulent reacting wakes or jets. Individual species can be followed with the mass spectrometer diagnostic as they are formed or destroyed in the jet. This capability is not limited to stable species, since the gas sampling is done in the jet flow itself at the point where the species are formed, and particle collisions before detection are minimized.

References

[1] Kantrowitz, A. and Grey, J., "A High Intensity Source for the Molecular Beam, Part I. Theoretical," *Review of Scientific Instruments*, Vol. 22, No. 5, 1951.

[2] Ashkenas, H. and Sherman, F., "The Structure and Utilization of Supersonic Free Jets in Low Density Wind Tunnels," *Rarefied Gas Dynamics*, 4th Symposium, edited by J. H. de Leeuw, Vol. II, 1966.

[3] Crist, S., Sherman, P. M., and Glass, D. R., "Study of the Highly Underexpanded Sonic Jet," *AIAA Journal*, Vol. 4, No. 1, Jan. 1966, pp. 68–71.

[4] Fenn, J. B. and Anderson, J. B., "Background and Sampling Effects in Free Jet Studies by Molecular Beam Measurements," *Rarefied Gas Dynamics*, 4th Symposium, edited by J. H. de Leeuw, Vol. II, 1966.

[5] Bossel, U., Investigation of Skimmer Interaction Influence on the Production of Aerodynamically Intensified Molecular Beams," Rept. AS 68-6, Aug. 1968, College of Engineering, Univ. of California at Berkeley, Berkeley, Calif.

[6] Chang, J., "Supersonic Molecular Beam Sampling Systems for Mass Spectrometri Studies of High Pressure Flow Systems," Research Rept. 326, April 1969, Avco Everett Research Lab., Everett, Mass.
[7] Laufer, J., "Turbulent Shear Flows of Variable Density," *AIAA Journal*, Vol. 7, No. 4, April 1969, pp. 706–713.
[8] Demetriades, A. and Doughman, E. L., "Mean and Intermittent Flow of a Self-Perserving Plasma Jet," *AIAA Journal*, Vol. 7, No. 4, April 1969, pp. 713–722.
[9] O'Conner, T. J., Comfort, E. H., and Cass, L. A., "Turbulent Mixing of an Axisymmetric Jet of Partially Dissociated Nitrogen with Ambient Air," *AIAA Journal*, Vol. 4, No. 11, Nov. 1966, pp. 2026–2032.
[10] Sutton, E., "The Chemistry of Electrons in Pure Air Hypersonic Wakes," *AIAA Journal*, Vol. 6, No. 10, Oct. 1968, pp. 1873–1883; also Research Rept. 266, July 1967; Avco Everett Research Lab., Everett, Mass.

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Nonequilibrium Flow Calculations for the Hydrogen Constricted Arc

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A nonequilibrium flow model has been formulated and solved numerically for conditions in an atomic hydrogen cascade arc. Solutions show that although thermal nonequilibrium effects are minor, the departure from chemical equilibrium is significant. Comparisons with results obtained from an equilibrium flow model reveal the deficiencies associated with such a model and parametric calculations reveal the effect of current, pressure, and radius on arc behavior.

Nomenclature

E = electric field intensity
I = arc current
I_p = ionization potential
k = Boltzmann's constant
n_e = electron number density
$\dot{n}_e$ = electron production rate
n_H = hydrogen atom number density
p = static pressure
P_I = diffusion of ionization energy
P_{rad} = radiative emission
q_{rad} = radiative wall heat flux
q_e = electron heat conduction
q_h = heavy particle heat conduction
q_w = total wall heat flux
R = tube radius
r = radial coordinate
S_{ec} = elastic collision energy transfer between electrons and heavy particles
T_e = electron temperature
T_h = heavy particle temperature
v_{amb} = ambipolar diffusion velocity
α_{rr} = radiative recombination coefficient
β = electron reflection coefficient
χ = ion reflection coefficient
σ_e = electrical conductivity

Introduction

THE wall stabilized cascade arc has been used extensively for the determination of high-temperature gas transport properties, for the simulation of high-speed aerodynamic phenomena, as a radiation source for photochemical processing, and as a means of energizing gas dynamic lasers. In support of these applications, much has been done to determine the thermochemical state of the arc gas. Earlier efforts involved the use of equilibrium flow models to predict arc temperature and species concentration profiles, as well as over-all heat-transfer effects.[1-3] More recently, however, comparisons between the equilibrium predictions and spectroscopic temperature measurements,[4,5] as well as comparisons with electric field intensity and wall heat-transfer data,[6] have suggested the existence of nonequilibrium effects. In particular, these comparisons have suggested the existence of a thermal nonequilibrium, for which there is a nonequipartition of translational energy between the electrons and heavy particles (each characterized by a separate kinetic temperature), and a chemical nonequilibrium, for which the Saha equation fails to predict species concentrations. Accordingly, more recent efforts to predict flow conditions in the cascade arc have considered the influence of thermochemical nonequilibrium conditions.[7-10]

The purpose of this study is to predict the thermochemical properties of the hydrogen arc and the extent to which nonequilibrium effects influence these properties. The behavior of hydrogen at elevated temperatures has astrophysical significance and bears directly on the simulation of Jupiter entry conditions.

Mathematical Model

Although conditions have been considered for both the entrance and asymptotic arc regions,[11] attention will be focused on the asymptotic results. In the asymptotic region, thermochemical conditions are uncoupled from hydrodynamic effects, and for prescribed arc operating conditions, the thermochemical variables depend only upon radius. It is assumed that the flow is laminar, steady, and axisymmetric, and that the electric field is directed only in the axial direction. The plasma is assumed to be quasineutral and is viewed as a perfect gas mixture of electrons, hydrogen ions, and neutral hydrogen atoms. The effect of neglecting the molecular species will be discussed later.

The governing differential equations may be derived by applying mass and energy conservation requirements to the

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