

Time-Dependent Analysis of Nonequilibrium Nozzle Flows with Complex Chemistry

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Theme

A NONEQUILIBRIUM, steady, quasi-one-dimensional nozzle flow with complex chemistry is computed by means of a time-dependent, finite difference technique. Results are given for a H—C—O—N chemically reacting mixture expanding through a rocket nozzle, and comparisons are made with the results of a steady flow kinetic analysis.

Contents

Nonequilibrium, steady, quasi-one-dimensional nozzle flows have been computed by means of a time-dependent, finite difference technique.^{1,2} In this technique, the fully coupled nozzle flow variables (pressure p , velocity u , temperature T and density ρ) and nonequilibrium properties (vibrational energy, chemical species) are computed throughout the nozzle in steps of time, starting from somewhat arbitrary initial conditions. The steady-state conditions, which are the desired result, are approached after a sufficient number of time steps.

This technique is now extended to the case of a complex chemically reacting mixture with many coupled fast and slow reactions. A specific case is chosen wherein the equilibrium reservoir conditions are produced from the combustion of N_2O_4 with 50% N_2H_4 /50% UDMH. The oxidizer to fuel ratio is 2.25 and the chamber pressure is 60 psia. The gas mixture flows through an axisymmetric nozzle with a 30° and 20° half-angle subsonic and supersonic section, respectively. The expansion is rapid enough so that nonequilibrium may prevail in the subsonic and supersonic portions of the nozzle. Viscous dissipation, diffusion, and thermal conduction are assumed to be negligibly small. Eleven chemical species (H, H_2 , O, O_2 , OH, H_2O , CO, CO_2 , N, N_2 and NO) and eleven reaction mechanisms are included in the computations. This case is the same as computed by Sarli et al.³ using a steady-state analysis. Also, reaction mechanisms and rate constants for the eleven binary shuffle and recombination reactions are from Ref. 3. Hence, a direct comparison of the numerical results is obtained.

For a specified nozzle shape $A = A(x)$ (where A is the cross-sectional area), initial values of flowfield variables ρ , u , T and the chemical composition are assumed at grid points spaced along the x -axis of the nozzle. If the flowfield variables are known at time t , then at each interior grid point new values

can be obtained at time $(t + \Delta t)$ from a series expansion in time,

$$g(t + \Delta t) = g(t) + \left(\frac{\partial g}{\partial t} \right)_{\text{ave}} \Delta t \quad (1)$$

where g is any flow variable or chemical composition and Δt is a small time increment chosen to satisfy certain stability criteria described in a subsequent section. Starting with the initial assumed variables at time $t = 0$, the flowfield is computed in steps of time from Eq. (1). At large values of time, the steady-state flowfield, which is the desired result, is obtained, where $(\partial g / \partial t)_{\text{ave}}$ approaches zero.

The time derivatives $(\partial g / \partial t)_{\text{ave}}$ are obtained from the unsteady quasi-one-dimensional continuity, energy, momentum and rate equations⁴ utilizing a modification² of the finite difference scheme of MacCormack.⁵

Increments of time Δt in Eq. (1) must satisfy two stability criteria,¹ the Courant-Friedrichs-Levy (CFL) criterion and a criterion governed by the speed of the nonequilibrium chemical processes such that

$$\Delta t \leq \beta \psi \quad (2)$$

where β is an empirical proportionality constant (unity for these computations) and ψ is the characteristic relaxation time for the fastest rate process.

Thirty-one total grid points located along the nozzle centerline are employed in this computation. Two grid spacing sizes are employed; 26 grid points with relatively fine spacing in the subsonic and throat regions and 5 grid points with coarse spacings in the remainder of the nozzle. This number of grid points was chosen as a matter of convenience and does not represent the minimum required for stability. The use of a fine grid spacing in the subsonic and low supersonic regions (where nonequilibrium effects are strong) enhances the numerical accuracy.

One of the advantages of the time-dependent technique is the ability to obtain a straightforward unified analysis of a nonequilibrium subsonic-supersonic flowfield. The spatial distribution of the hydrogen atom mole fraction shown in Fig. 1 is representative of the unified analysis. Behavior of the hydrogen atom mole fraction is shown at various dimensionless times starting from the initial distribution (essentially frozen at reservoir conditions) and proceeding to the steady-state solution at $t' = 1.741$. (Here t' is time nondimensionalized by the ratio of nozzle length and reservoir sound speed). Chemical nonequilibrium effects are seen to be present in the subsonic region near the throat.

A comparison of the present analysis with the steady flow kinetic analysis of Sarli et al.³ is presented in Figs. 2 and 3. Although only the supersonic portion of the nozzle is shown in these figures, both techniques consider upstream nonequilibrium effects. The agreement between the two methods for the spatial distributions of vacuum specific impulse, static temperature and chemical species is generally very good.

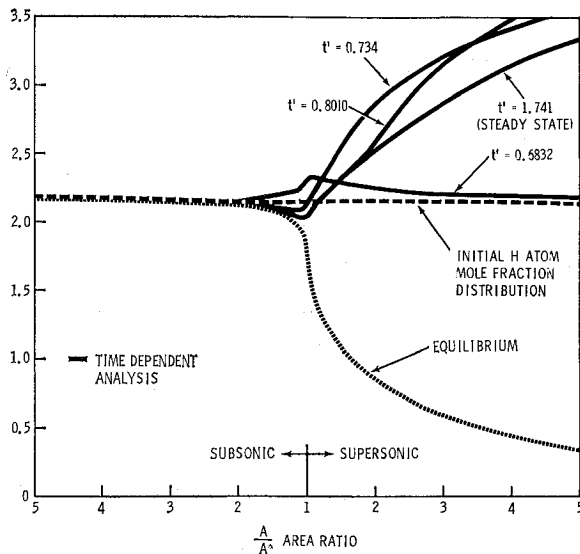
The present analysis and results indicate that the time-dependent technique of Refs. 1 and 2 can be applied to complex chemistry in a straightforward manner.

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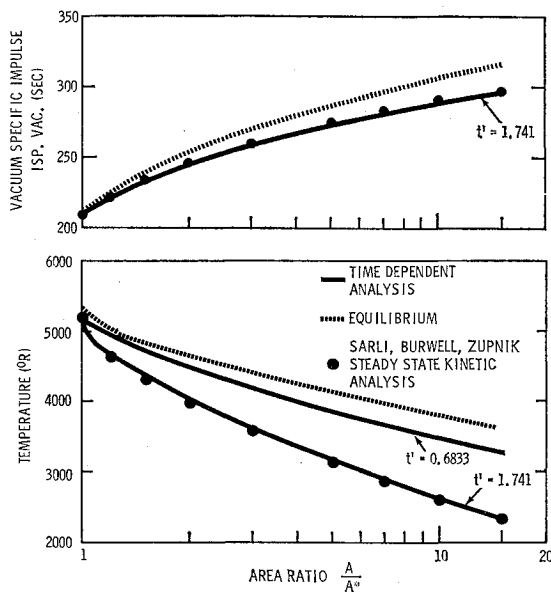
Index categories: Reactive Flows; Nozzle and Channel Flow.

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1 Transient and steady-state variations of hydrogen atom mole fraction through the nozzle.



2 Spatial variations of vacuum specific impulse and temperature.

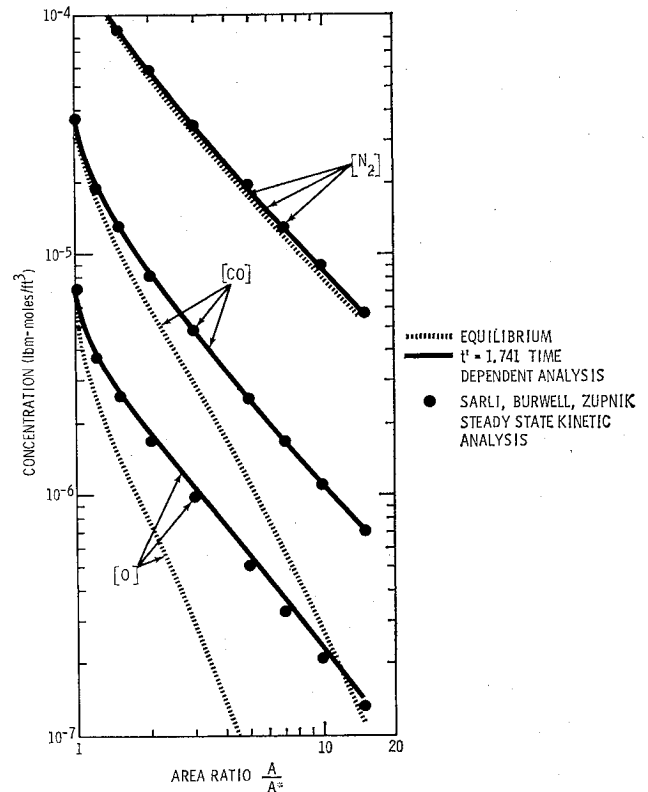


Fig. 3 Comparisons of molecular and atomic concentration profiles.

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