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REACTING FLOWS USING A SPECTRAL MULTI-DOMAIN TECHNIQUE**

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An Analysis of Artificial Viscosity Effects on Reacting Flows Using a Spectral Multi-Domain Technique

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Standard techniques used to model chemically-reacting flows require an artificial viscosity for stability in the presence of strong shocks. The resulting shock is smeared over at least three computational cells, so that the thickness of the shock is dictated by the structure of the overall mesh and not the shock physics. A gas passing through a strong shock is thrown into a nonequilibrium state and subsequently relaxes down over some finite distance to an equilibrium end state. The artificial smearing of the shock envelops this relaxation zone which causes the chemical kinetics of the flow to be altered. This paper presents a method which can investigate these issues by following the chemical kinetics and flow kinematics of a gas passing through a fully resolved shock wave at hypersonic Mach numbers. A nonequilibrium chemistry model for air is incorporated into a spectral multi-domain Navier-Stokes solution method. Since no artificial viscosity is needed for stability of the multi-domain technique, the precise effect of this artifice on the chemical kinetics and relevant flow features can be determined.

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1. INTRODUCTION

Since the inception of the design of the Space Shuttle more than 15 years ago, there has been considerable progress in prediction methodologies. We are beginning to see increasing sophistication in chemically reacting flow methods which involve nonequilibrium and two-temperature chemical kinetics [1,2]. To successfully couple a nonequilibrium chemistry model with the flow kinematics, we must first fully understand the impact the numerical algorithm has on the problem at hand. Such an investigation has not been researched to date; this work addresses fundamental questions relevant to such understanding.

The standard technique used to model chemically reacting or non-reacting flows are finite-difference or finite-volume methods. One common feature shared by both techniques is the artificial viscosity needed in the presence of strong shocks. The effect that the artificial viscosity has is to smear the shock over at least three computational cells. The size of these cells is not directed by the shock physics but by the structure of the overall mesh.

When air passes through a strong shock wave, there follows a conversion of energy of directed translational motion into other forms of energy such as translation, rotation, vibration, and dissociation. Since the temperature of a gas depends on the energy of translation, when energy is transferred into this form, the temperature of the gas rises. If, at a later time, a portion of the energy of translation is converted into other modes, the temperature falls. Because of differences in the magnitude of the time required for the different processes to absorb their equilibrium amount of energy, considering them to occur separately and consecutively results in a good approximation [5]. The variation of temperature from its free-stream value to its value following establishment of thermal equilibrium can, therefore, be represented as in the schematic given in Fig. 1 [3]. Station (1) represents conditions in the free stream ahead of the shock wave where the temperature is low enough that vibration of the molecules is not appreciably excited. Rotation of the molecules is, however, completely excited. Station (2) represents conditions in the free stream ahead of the shock wave where the temperature is low enough that vibration of the molecules is not appreciably excited. Rotation of the molecules is, however, completely excited. Station (2) represents conditions behind but very close to the shock wave. The thermal jump across the shock wave throws the translational and rotational degrees of freedom temporarily out of equilibrium, but only a few molecular collisions are required to establish equilibrium not only of the translational but also of the rotational degrees of freedom. Adjustment of the vibrational degrees of freedom occurs between stations (2) and (3). This process requires a number of collisions (or a time or distance) that are large compared with that required for adjustment of translation and rotation, but are small compared with that required for establishment of dissociation equilibrium. At station (3), vibration is fully established but dissociation is only beginning. At station (4), sufficient time has elapsed for the dissociation of oxygen to reach equilibrium; and,

at station (5), the dissociation of nitrogen is in equilibrium and the temperature has reached its equilibrium value. These relaxation pathways are transition zones which initiate the chemical kinetics which follow. The pertinent questions are: Does the artificial smearing of the shock envelop the transition region; and if so, is the distribution of energies and chemical composition significantly altered so as to affect the chemical kinetics of the flow.

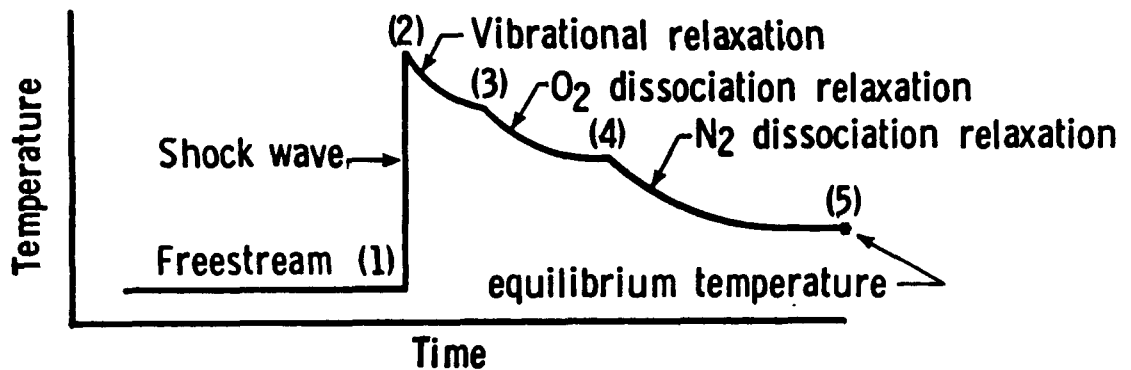


Fig. 1. Schematic of relaxation zones for nonequilibrium air.

Fig. 2 is a plot of data accumulated from shock-tube experiments [4,5,6,7]. Shock thickness and relaxation path lengths are plotted against Mach number in air. The data corresponds to shock thicknesses and relaxation path lengths which exist at an altitude of 120,000 feet. As can be

seen, the shock thickness at this altitude is within two or three orders of magnitude of these relaxation lengths. A typical calculation easily smears a shock over several orders of magnitude which is sufficient to obliterate this important region. Though it is possible with standard finite-difference techniques to resolve the shock sufficiently so that vibrational relaxation can be modeled, a calculation for more than just a very small region will be computationally to expensive. To make such a calculation practical for full-scale application the needed resolution must be attainable on a tractable grid. At the very least, present day computations of chemically-reacting flows should be paralleled by fundamental studies of the effects factors inherent in the algorithm have on the relevant physics.

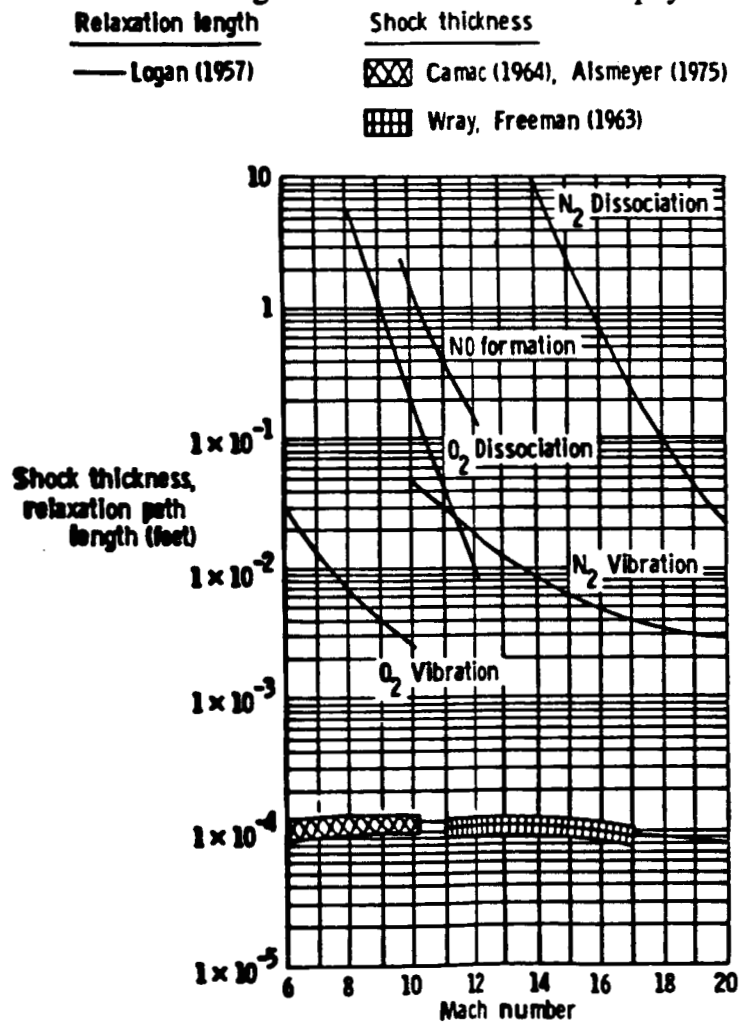


Fig. 2. Comparison of relaxation path lengths and shock thicknesses; altitude = 120,000 feet.

A methodology well suited for carrying out such a study is the spectral multi-domain technique [7]. One of the strongest properties of spectral methods is their exponential rate of convergence and high-order accuracy on relatively coarse meshes [8]. Extensions of their application to include capturing regions of high gradient and modeling complex geometries has recently been attainable due to the spectral multi-domain technique developed by Macaraeg and Streett [9]. The multi-domain

technique interfaces regions with independent discretizations, while maintaining spectral accuracy and an exponential rate of error decay. Adjoining regions are interfaced by enforcing a global flux balance which preserves high-order continuity of the solution. This interface technique maintains spectral accuracy, even when mappings and/or domain sizes are radically different across the interface. Such advantages are needed when computing chemically reacting flows, which can display widely disparate temporal and spatial scales due to fast chemical reaction as opposed to the macroscopic scales associated with the hydrodynamics.

2. MULTI-DOMAIN SPECTRAL TECHNIQUE

A number of other spectral domain decomposition techniques have appeared in the literature. For example, the spectral element method which applies finite element methodology using Galerkin spectral discretization in the variational formulation within elements is a popular technique [10,11]. One drawback with this technique is that it utilizes a split Galerkin-collocation discretization which restricts its application to convection-diffusion problems for incompressible flows. The spectral element method in practice is used in a manner similar to classical finite element techniques: low-order internal discretization using many elements with no internal stretchings to improve resolution. In addition each element contains the same number of collocation points. Other domain decomposition techniques involve explicit enforcement of C1 continuity across the interface [12,13]. It is not clear how well these techniques perform for strongly convection-dominated problems; the second author's experience with such techniques [14] has shown them to be not entirely satisfactory.

The multi-domain spectral technique overcomes the above restrictions by splitting the domain into regions with independent collocation discretizations, each of which preserve the advantages of spectral collocation, and allow the ratio of the mesh spacings between regions to be several orders of magnitude higher than allowable in a single domain. The partitioning results in three classes of points: the interior points where collocation of the equation is applied, boundary points where the physical boundary conditions are applied, and interface points which satisfy a global flux balance across adjoining sub-domain and preserve high-order continuity of the solution. The global flux balance is imposed in terms of a spectral integral of the discrete equations across adjoining domains. In the multi-dimensional case this integration is performed along the coordinate line perpendicular to the interface. If adjoining domains have coordinate lines perpendicular to the interface which do not align, the solution from the domain with the lesser number of points are spectrally interpolated from the fine grid onto the coarse grid. To close the equation set, continuity of the solution and the flux is imposed at the interface. The total system of interface relations has a block structure-- each block spanning a single interface between a pair of adjoining domains. Since the discretizations interior to each domain are solved uncoupled from each other and since the interface relation has a block structure, the solution scheme can be adapted to the particular requirement for each domain. Iterative and noniterative schemes have been developed to solve the combined interior/interface system. Details of the algorithm as well as comparisons between the present method, spectral element, and single domain collocation are given in ref. 7.

3. NUMERICAL MODEL

The above technique will model the chemical kinetics and flow kinematics of a nonionized air mixture (O_2 , N_2 , NO , O , and N) passing through a fully resolved shock wave, thus alleviating the need for artificial viscosity. The governing equations are the quasi-one dimensional Navier-Stokes equations [15], and species conservation equation [1]. The quasi-one dimensional form is used to provide an artifice for controlling the shock location in the physical space for this otherwise indeterminate problem. The equations are nondimensionalized by dividing the state and transport parameters by their dimensional free stream values.

The viscosity of each of the individual species are calculated from a curve fit relation [16]. Similarly, curve fits are used to obtain specific heats, internal energies, and enthalpies [17,18]. The thermal conductivity of each specie is calculated from the Eucken semi-empirical formula using the specie's viscosity and specific heat. Appropriate mixture rules are next used to obtain the above transport properties of the mixture [19]. Experimental values of bulk viscosities, as obtained from acoustical interferometry and related experiments, are taken from Truesdell [20].

In the present work, the diffusion model is limited to binary diffusion with the binary diffusion coefficients specified by the Lewis number. The value of the Lewis number used is 1.4.

The temperature range under study will not exceed 8000 degrees kelvin, for conditions at an altitude of approximately 190,000 feet. Therefore, ionization reactions, which occur at roughly 9000 degrees kelvin, are not included. The chemical reactions utilized for the nonionized air mixture are impact dissociation and exchange reactions. The seventeen reactions included in the present study can be found in ref. 1, which also lists ionization reactions. The constants needed to evaluate reaction rates are given in ref. 2.

Initial conditions are obtained from a spectral multi-domain code for solution of the Navier-Stokes equations with equilibrium chemistry, written for the above problem. These governing equations may be found in ref. 15. Transport properties are obtained in the manner previously discussed. The routines of ref. 17 generalized for air are used to obtain equilibrium concentrations.

4. NUMERICAL ALGORITHM

The multi-domain discretization involves three independent subdomains, with the shock located in the center subdomain. Shock jump conditions are obtained by an iterative procedure to solve the Rankine-Hugoniot relations for real air.

A direct inversion of the coupled system is utilized to obtain a fully implicit method. The conserved variables are written in delta form, and a pseudo time iteration using backwards Euler is utilized to obtain the steady state solution. Because of the large rank and ill-condition of the Jacobian matrix, iterative improvement of the Gaussian elimination solution was found to be required.

5. METHOD VERIFICATION

Validity of the multi-domain Navier-Stokes algorithm is demonstrated by comparison with experiment. A low-density wind tunnel study of shock-wave structure and relaxation phenomena in gases was conducted by Sherman [21]. The experiment measured shock wave profiles recorded in terms of the variation in the equilibrium temperature of a small diameter wire oriented parallel to the plane of the shock, as the wire is moved through the shock zone. Free stream Mach number is 1.98. For this test case, a Navier-Stokes spectral multi-domain calculation is performed for a perfect gas with temperature dependent properties and a nonzero bulk viscosity corresponding to air [20]. A comparison with experimental temperatures normalized by the free stream temperature versus normalized distance is given in Fig. 3. The experimental data points are represented by the open symbols. The numerical results fall within a symbol width of the data. The multi-domain technique utilized three domains. The center domain, located between $x = -.15$, and $x = 0.3$, contains 21 points; the outer domains contain 11 points each. The computational domain spans -1 to 1. The unit Reynolds number of the flow is 80. A calculation for a unit Reynolds number of 1000 is given in Fig. 4, showing the ability of the method to accurately resolve strong gradients without numerical oscillations. The plot is of Mach number versus normalized distance. Three domains are again used; the center domain contains 17 points, the outer domains contain 11 points each. The interfaces are located at $-.15$ and $-.1$.

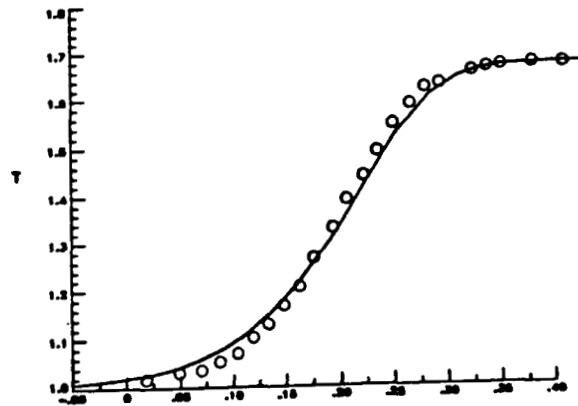


Fig. 3. Comparison of multi-domain Navier-Stokes calculation with experimentally obtained temperatures; $M_\infty = 1.98$, $Re = 80$. Discretization 11/21/11, interfaces at $-.15$ and 3 .

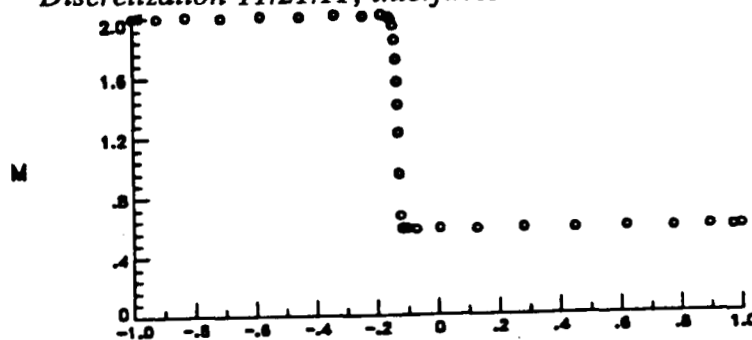


Fig. 4. Computed solution for $Re = 1000$; discretization 11/17/11, interface at $-.15$ and $-.1$.

6. RESULTS

The case to be discussed with respect to effects of nonequilibrium assumptions on the flow/chemistry is for $M_\infty = 11.0$, $T_\infty = 350\text{K}$, and $\rho_\infty = 6 \times 10^{-8} \text{ g/cm}^3$. These conditions invoke primarily O_2 dissociations, with N_2 dissociations just beginning. Temperatures are not yet high enough for ionization to occur, so vibrational energy modes remain unexcited.

Typical discretizations used in this study were 15, 27 and 33 points in the upstream, middle and downstream domains, respectively. The backward-Euler implicit time-stepping algorithm typically required less than 2000 iterations to converge from an equilibrium starting solution, with at least an eight order of magnitude reduction in maximum residual.

It is interesting to note the effect of downstream boundary conditions of the chemical species on the numerical results. Two boundary conditions are compared in Fig. 5. The first involves imposing the equilibrium end state concentrations corresponding to the post shock temperature and density values from the equilibrium jump conditions. The second involves a zero gradient boundary condition on species' concentrations. The plot is of the log of the concentration in the relaxation zone versus normalized distance behind the shock. It is evident that the extrapolation condition leads to a smooth profile of concentrations down to a desired end state, whereas an imposed equilibrium end state causes oscillations in the numerics and a resulting discontinuity between the imposed equilibrium end state and the pathway chosen by the chemical kinetics calculation.

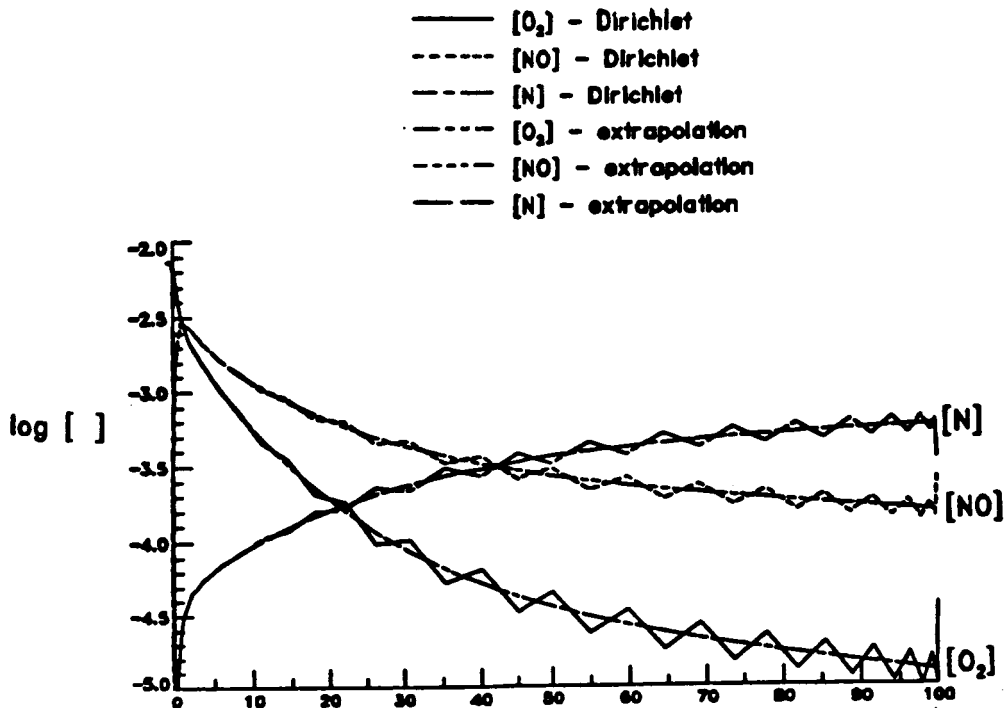


Fig. 5. Species concentrations in the relaxation zone for both Dirichlet (imposed equilibrium endstate) and extrapolation boundary conditions.

To test the effect of the extrapolation boundary conditions on the chemical kinetics, a comparison is made between a computation for which the post-shock physical domain is long enough to allow the concentrations to relax to their final values, and one in which the domain is severely truncated. The results for $[O_2]$ and $[O]$ are shown in Fig. 6, with the truncated-domain $([-1,1])$ solution represented by symbols, and the extended-domain $([-1,120])$ solution shown as lines. As can be seen, the profiles are identical.

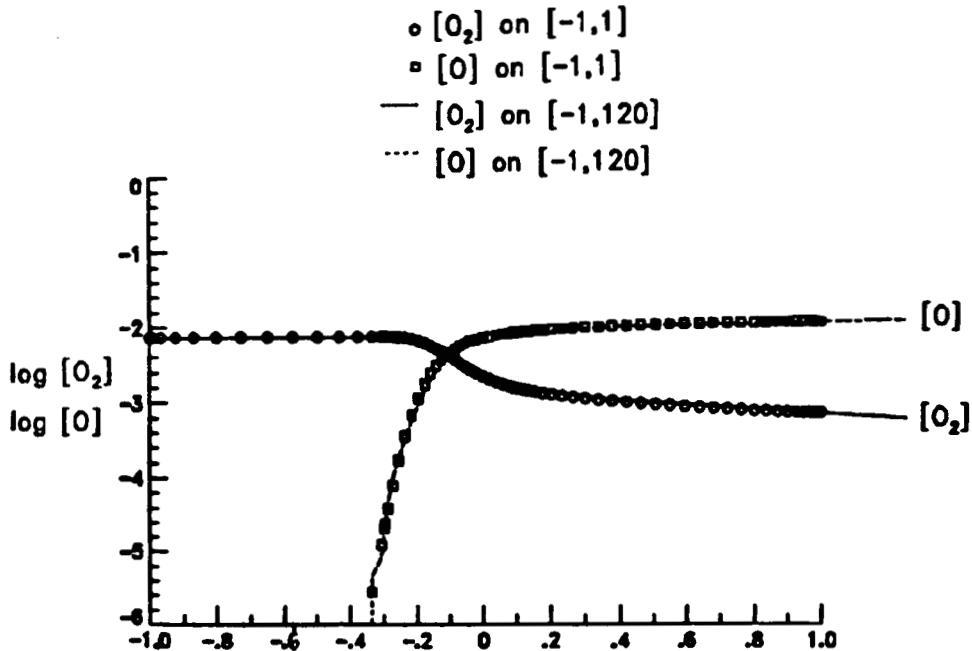


Fig. 6. Comparison of $[O_2]$ and $[O]$ in the relaxation zone spanning $[-1,1]$ and $[-1,120]$.

The study of the effect of artificial viscosity on the flow physics was carried out by adding the equivalent of second-order artificial viscosity to the momentum, energy, and species' concentration equations. The amount of artificial viscosity introduced was such that the shock was spread out to a thickness about three orders of magnitude wider than the fully-resolved no artificial viscosity solution. This width was chosen to represent the grid spacing of a typical shock-capturing computation on a full-scale configuration, such as that mentioned in the Introduction. Figures 7a. and 7b. show the Mach number and temperature profiles for the resolved-shock and smeared-shock cases, respectively; note that the entire physical domain is shown in Fig. 7b, whereas only the near-shock region on a greatly expanded scale is plotted in Fig. 7a. For the resolved-shock case, endpoints are at -1 and 200, and interface points are at -.3 and .1. The interface locations for the smeared shock case are at 65 and 100, with endpoints at 0 and 270. The most important feature to note in comparing these profiles is the 20% reduction in the temperature overshoot as a result of the artificial viscosity. We conjecture that this is not the result of simple

smearing, but is produced by the change in the relative magnitude of the spatial scales of the flow kinematics and chemical kinetics. The temperature overshoot is produced by the conversion of kinetic energy to thermal energy, on a scale too small for the chemistry to respond. Thus the near-shock chemistry is essentially frozen, and the ratio of enthalpy to internal energy remains near its freestream value. The chemical reactions then begin to respond on their own scale, as dictated by the reaction rate constants used in the model. A fraction of this released thermal energy is absorbed by the reactions, lowering the temperature. When the shock is smeared, the release of thermal energy occurs on a scale nearer that on which the reactions operate, and therefore some of this energy is absorbed by the reactions while the release is still taking place. This reduces the overshoot in temperature.

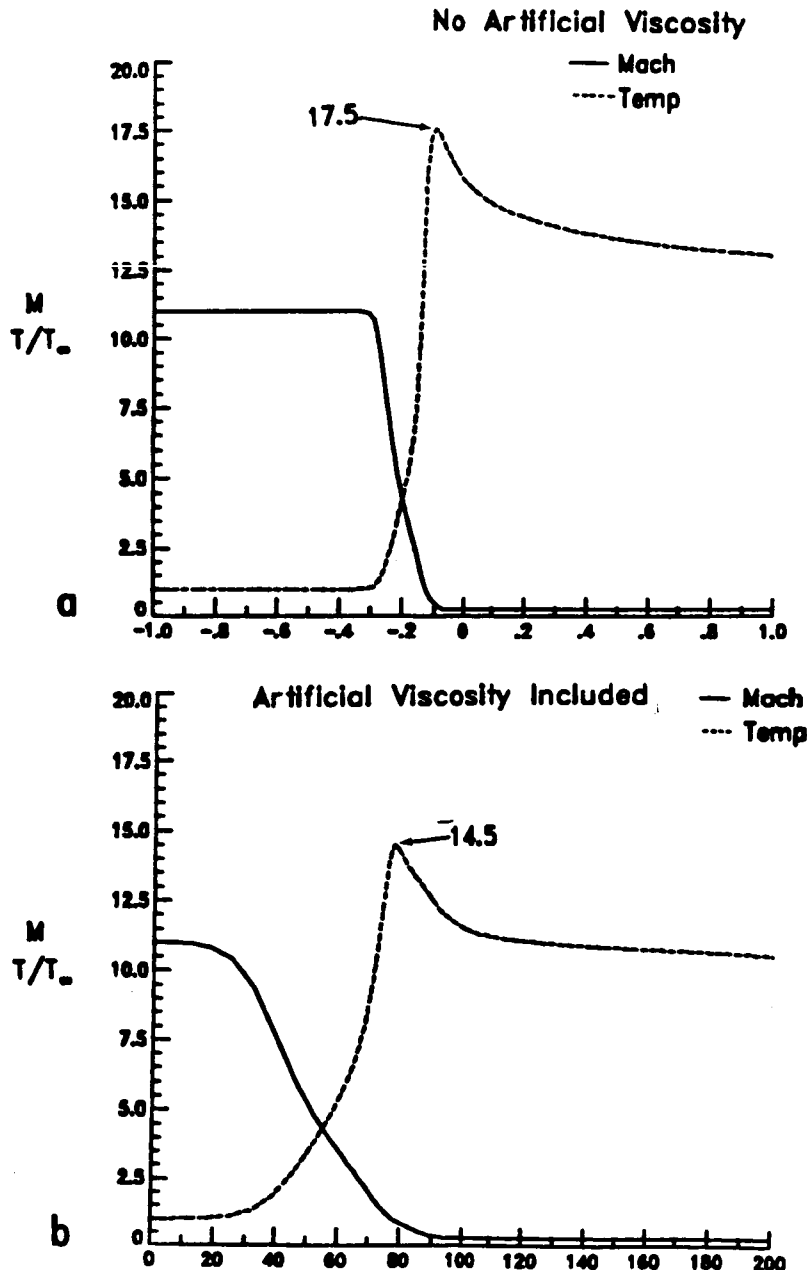


Fig. 7. Comparison of temperature and Mach number profiles for calculations a) without artificial viscosity, and b) with artificial viscosity.

Simple smearing of the shock from the artificial viscosity cannot account for this effect as can be realized by considering an equilibrium calculation. For such a calculation, only one spatial scale exists, and is dictated by the Reynolds number. Thus a change in scale or a change in Re are equivalent. Introduction of second-order artificial viscosity may, of course, be looked at as lowering the effective Re of a calculation. Thus any change in the shock profile by the introduction of artificial viscosity which cannot be accounted for by a simple scale change must be attributed to an alteration of the interplay between flow kinematics and chemical kinetic scales. This effect can be expected to strengthen with increasing Mach number.

For the Mach 11 case considered here, although the path along which the chemistry relaxes is significantly altered in the near-shock region, the chemical end states from the computations with and without artificial viscosity are within 3-4% of each other. This can be seen in Figs. 8a,b and 9a,b, which show the profiles of $[O_2]$ and $[O]$ (Figs. 8a,b) and $[N]$ and $[NO]$ (Figs. 9a,b) in the relaxation zone. This is not to say, however, that this situation will always occur especially for higher Mach numbers where vibrational excitation (ionization) occurs. The reduction in the temperature overshoot could result in a large enough change in the relaxation path that the end state could be affected. For example, ionization reactions will not occur if artificial viscosity decreases this overshoot so that temperatures are not sufficiently high to initiate its onset.

7. DISCUSSION

Although smooth, accurate and consistent solutions have been obtained for the species' concentrations in the post-shock region, which is the region of interest here, we feel the solutions are not entirely satisfactory in the upstreams region and in the shock. The difficulty is that the range over which several of the species' concentrations vary is too large to be accurately represented, given the Cray single-precision computations employed. Although iterative improvement is used in the Jacobian inversion of the time-stepping scheme to reduce the effects of finite word length, the usable dynamic range of the solution was limited to about six orders of magnitude. In the solution for $[O]$, for example, the end state concentration is about 10^{-2} ; the $[O]$ solution in the free stream, however, oscillates at about $\pm 10^{-8}$, where the equilibrium concentration should be about 10^{-34} . This extremely small oscillation disappears in the shock region when reactions begin to take place, but it is still something of an annoyance. Fig. 3 of reference [1] also shows evidence of this difficulty in the near-shock region. We are investigating recasting species' concentration equations in terms of the logarithm of the concentrations, to better resolve the entire dynamic range of the solution.

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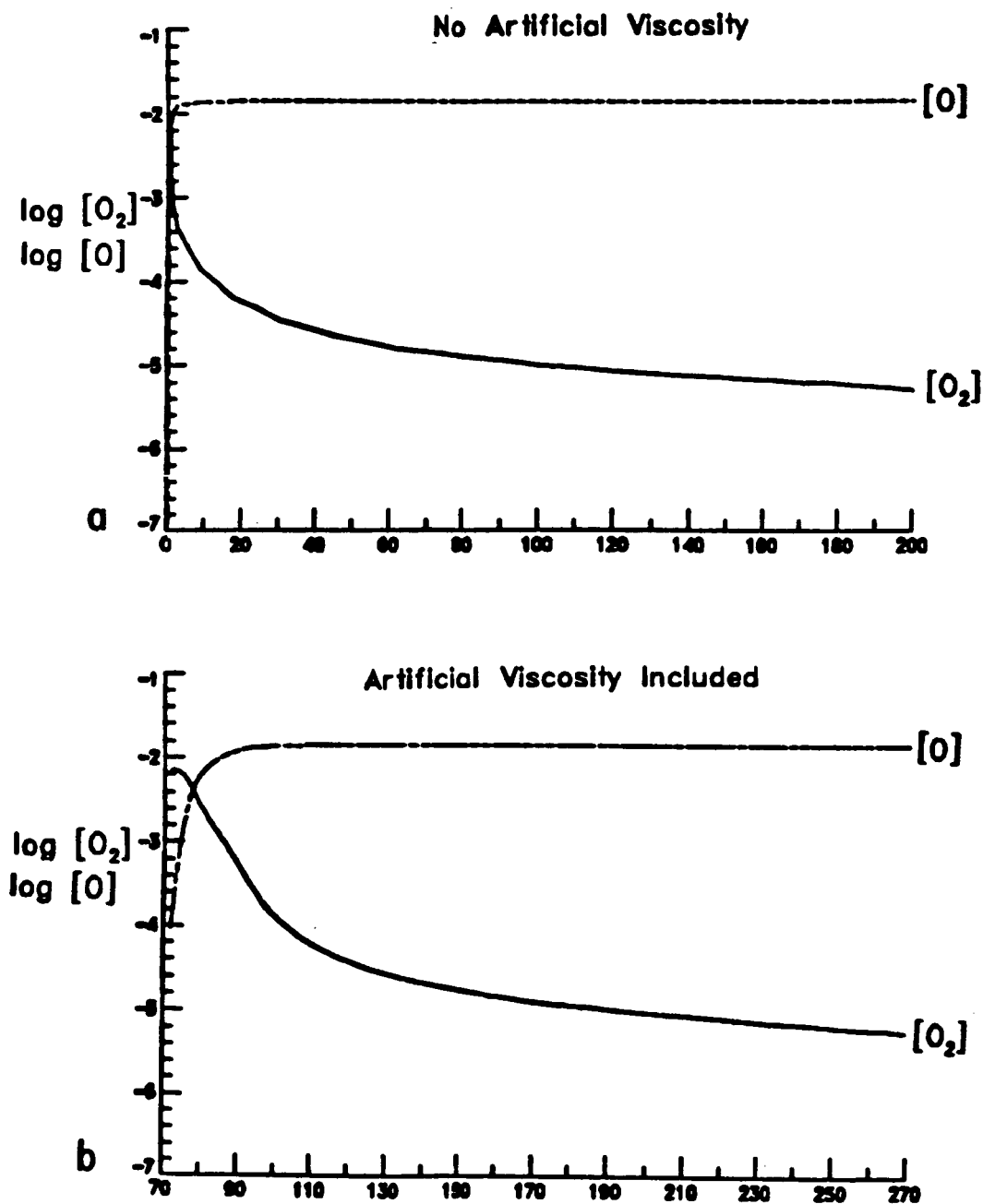


Fig. 8. Comparison of relaxation pathway for [O₂] and [O] for calculations a) without artificial viscosity, and b) with artificial viscosity.

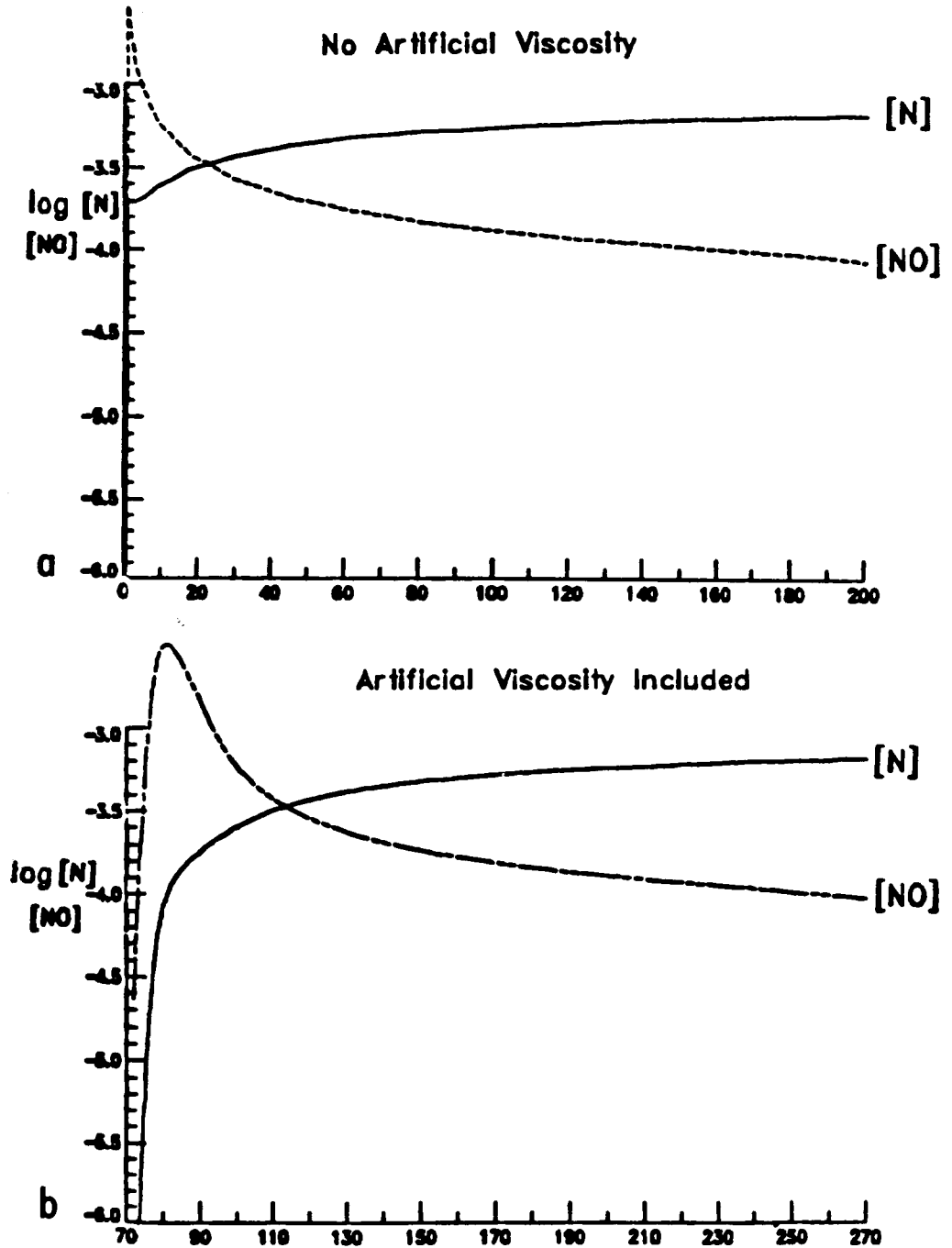


Fig. 9. Comparison of relaxation pathway for $[N]$ and $[NO]$ from calculations
a) without artificial viscosity, and b) with artificial viscosity.

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