

# AIAA'87

**AIAA-87-2549-CP  
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Two-Dimensional  
Viscous, Unsteady Dissociating  
Nitrogen Flows**

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**AIAA 5th Applied Aerodynamics  
Conference**

**August 17-19, 1987**

**Monterey, California**

NUMERICAL SIMULATION OF TWO-DIMENSIONAL VISCOUS UNSTEADY  
DISSOCIATING NITROGEN FLOWS

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ABSTRACT

An explicit, time accurate, predictor-corrector scheme, similar to MacCormack's has been used to simulate unsteady non-equilibrium, laminar chemically reacting flows. A zonal approach, along with non-structured boundaries, allows computation of internal and external flow with the same computer code. Results for equilibrium flows of dissociating, vibrationally relaxing nitrogen in a rectangular chamber are presented.

NOMENCLATURE

C atomic concentration of N  
 $C_p$  specific heat at constant pressure  
 D computational domain or subdomain also diffusion coefficient)  
 $E_{vib}$  vibrational energy of diatomic molecules  
 h enthalpy per unit mass  
 $h_t$  total enthalpy per unit mass  
 I identity tensor  
 k reaction rate constant  
 K equilibrium constant  
 $L_e$  Lewis Number:  $\frac{\rho C_p D}{\lambda}$   
 m specie molar mass  
 $\bar{m}$  mixture molar mass:  $\bar{m} = \left( \sum_{s=1}^{m_s} m_s X_s \right) / \left( \sum_{s=1}^{n_s} X_s \right)$   
 $\underline{n}$  unit vector normal to a surface (pointing to the exterior)

$n_s$  number of species  
 p thermodynamic pressure  
 $P_r$  Prandtl number  $P_r = \frac{\mu C_p}{\lambda}$   
 q total heat flux  
 R Boltzmann constant  
 $S_1$  set of indices of monoatomic species  
 $S_2$  set of indices of diatomic species  
 T absolute temperature

$\underline{u}$  fluid velocity  
 $\underline{u}'$  grid displacement velocity  
 v specific volume  
 X concentration  
 $\dot{X}_{react}$  species source term due to chemical reactions

Greek Letters

$\Delta H'_{fi}$  (or  $\Delta H_{fi}$ ) enthalpy of formation of diatomic (monoatomic) specie  
 $\theta_v$  characteristic temperature for vibration of diatomic specie  
 $\lambda$  thermal conductivity;  $\lambda = \lambda_l + \lambda_{tu}$   
 $\mu$  coefficient of shear viscosity;  $\mu = \mu_l + \mu_{tu}$   
 $\mu_B$  coefficient of bulk viscosity  
 $\rho$  density  
 $\tau$  viscous stress tensor  
 $\tau_v$  vibrational relaxation time

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Symbols

$\frac{d}{dt}$	Lagrangian derivation
$\frac{\partial}{\partial t}$	Eulerian derivation
$\frac{\delta}{\delta t} = \delta_t$	time derivative following a point p moving at a velocity $\underline{u}'$
$\times$	vector product
$\otimes$	tensor product
$\Pi$	product
$     $	norm of a vector

Subscripts

(eq)	equilibrium
f	formation
s	monoatomic or diatomic specie
t	total

Superscript

o	initial
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INTRODUCTION

The interest in accurate prediction of all aspects of hypersonic flows around configurations of arbitrary shape has recently been enticed by several projects [1], [2], [3].

At the very high Mach numbers, behind a strong shock, air is dissociating, vibrationally excited and out of equilibrium. Moreover, radiative effects can become very important [4], and ionization can appear. Very few experimental data are available, and very few facilities are able to reach the operating range of these new vehicles. Thus, one has to use sophisticated computer codes to predict the complex aerothermal fields around such hypersonic vehicles from the limited amount of data available. Perfect (non reacting) equilibrium flow computations are available [5], [6], [7] and have been successfully compared with experimental data for simple geometries [8]. Non equilibrium reactive flow computations [9], with radiative effects [10], have been recently made possible because of the availability of new supercomputers. These computations are very time consuming, and some attempts have been made to apply parabolized Navier Stokes codes [11], [12], to non equilibrium flows.

Park [13] has shown the need for a two temperature model for the correct representation of chemical rates. Most of the available codes do not take into account vibrational relaxation, thus limiting their range of applications or their accuracy.

The code that we present in this paper gives the time dependent solution for a two dimensional flow of multicompositional reacting gas. It takes into account vibrational relaxation of diatomic molecules and non equilibrium chemistry. The code is able of treating internal or external laminar flows.

Provision has been made for possible displacements of the grid points, allowing the use of optimal grids [14]. An explicit Mac Cormack scheme [15] has been chosen, for its suitability for vector computation and its high time accuracy. The use of non structured boundaries as well as a zonal approach, allow for more versatile applications.

GOVERNING EQUATIONS

When the body forces, electromagnetic and radiative effects are neglected, then the species continuity, momentum, and energy equations can be written in a compact form, as:

$$\frac{\delta X_i}{\delta t} + \nabla \cdot (X_i \underline{u}) - \underline{u}' \cdot \nabla X_i = \nabla \cdot [\rho D_i \frac{X_i}{\rho}] + \dot{X}_{i,react} \quad i=1, \dots, n_s \quad (1)$$

$$\frac{\delta \rho \underline{u}}{\delta t} + \nabla \cdot (\rho \underline{u} \otimes \underline{u} + P \underline{I} - \underline{\tau}) - \underline{u}' \cdot \nabla \rho \underline{u} = 0 \quad (2)$$

$$\frac{\delta \rho e_t}{\delta t} + \nabla \cdot (\rho \underline{u} e_t + \underline{q} + P \underline{u} - \underline{\tau} \cdot \underline{u}) - \underline{u}' \cdot \nabla \rho e_t = \sum_{i \in S} \nabla \cdot ( (\rho h_i) (\frac{\rho D_i}{X_i} \frac{X_i}{\rho}) ) + \Delta H_{react} \quad (3)$$

This system must be complemented by the vibrational energy equations, for each diatomic specie

$$\frac{\delta E_{vib}^i}{\delta t} + \nabla \cdot (E_{vib}^i \underline{u}') - \underline{u}' \cdot \nabla E_{vib}^i = \frac{E_{vib}^i (eq) - E_{vib}^i}{\tau_v} \quad (4)$$

The variables that we use are:  $X_i, \rho \underline{u}, \rho e_t,$

$$E_{vib}^i.$$

This system needs also the following state relations and definitions:

$$P = ( \sum_{s=1}^{n_s} X_s ) RT \quad (5)$$

$$\rho = \sum_{s=1}^{n_s} m_s X_s \quad (6)$$

$$\underline{\tau} = \mu (\nabla \underline{u} + \nabla \underline{u}^t) + (\mu_B - \frac{2}{3}\mu) (\nabla \cdot \underline{u}) \underline{I} \quad (7)$$

$$i \in S_1 (h_i) \quad \rho h_i = X_i (\frac{5}{2} RT) + m_i X_i \frac{u^2}{2} \quad (8)$$

$$i \in S_2 (h_i) \quad \rho h_i = X_i (\frac{7}{2} RT + E_{vib}^i) + m_i X_i \frac{u^2}{2} \quad (9)$$

$$(\Delta h) \Delta H_{react} = \sum_{i=1}^{n_s} X_{i,react} \Delta H_{fi} \quad (10)$$

$$(h_t) \rho h_t = \sum_{i=1}^{n_s} \rho h_i \quad (11)$$

These governing equations include the term

$$\underline{u} \cdot \nabla \{ \underline{x}_i, \rho \underline{u}, \rho e_t, \underline{E}_{vib}^i \}^T.$$

This term is similar to the one introduced by Brackbill [16], and allows movements of the computational grid as function of time. Optimal solution adaptive composite grids could be used, such as the one developed by Kennon, Dulikravich and Carcaillet [14].

#### THERMODYNAMIC AND TRANSPORT PROPERTIES

The specific heat of the mixture is obtained from:

$$C_p = \sum m_i X_i C_{pi} \quad (12)$$

Where  $C_{pi}$  is the specific heat at constant pressure of component  $i$  at the temperature  $T$  of the mixture.  $C_{pi}$  is obtained by interpolation of thermodynamic data from Miner and Lewis [17].

For each specie, the viscosity  $\mu_i$  is given by a curve fit relation:

$$\mu_i = 10^{-1} \exp(C_i) T^{(A_i \ln T + B_i)} \quad (\text{kg m}^{-1} \text{s}^{-1}) \quad (13)$$

$T$  is the absolute temperature, in K,  $\mu_i$  the viscosity;  $A_i$ ,  $B_i$  and  $C_i$  are given by Miner and Lewis [17]. Then,  $\mu$  for laminar flows is obtained by Wilke's semi-empirical relations

$$\mu = \sum_{i=1}^n \frac{x_i \mu_i}{\sum_{j=1}^n x_j \phi_{ij}} \quad (14)$$

and

$$x_i = X_i \bar{m}/m_i,$$

$$\phi_{ij} = [1 + (\frac{\mu_i}{\mu_j})^{1/2} (\frac{m_i}{m_j})^{1/4}]^2 [\sqrt{8} (1 + \frac{m_i}{m_j})^{1/2}]^{-1} \quad (16)$$

Similarly, as for the determination of the viscosity, we obtain the coefficient of heat conductivity  $\lambda$  by computing

$$\lambda_i = \frac{\mu_i R}{m_i} \left( \frac{C_{pi} m_i}{R} + \frac{5}{4} \right) \quad (17)$$

for each specie  $i$ .

Then, the total thermal conductivity for laminar flows is

$$\lambda = \sum_{i=1}^n \frac{x_i \lambda_i}{\sum_{j=1}^n x_j \phi_{ij}} \quad (18)$$

The diffusion coefficient is obtained from

$$D_i = \frac{\lambda}{\rho C_p} Le_i, \quad (19)$$

where  $Le_i$  is the Lewis number of specie  $i$  assumed to be constant and equal to 1.4.

#### CHEMISTRY

Near a strong shock wave, the vibrational temperature is not at its equilibrium value and can be very different from the translational temperature. Park [13] has shown the importance of the correct evaluation of this temperature for the purpose of computing the chemical rate coefficients. An approximation of the model of vibrational relaxation of Landau and Teller, detailed by Vincenti and Kruger [18], has been adopted. In this model the relaxation time  $\tau_v$  is given by

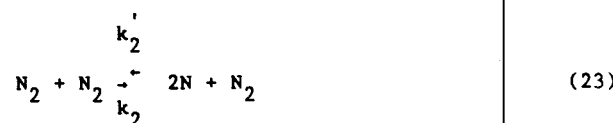
$$\tau_v = C \frac{\exp(k_2/T)}{P} \quad (20)$$

and the equilibrium vibrational energy is

$$E_{vib}^{(eq)} = R \frac{\theta_v}{\exp(\frac{\theta_v}{T}) - 1} \quad (21)$$

The values of constants  $C$ ,  $k_2$  and  $\theta_v$  can be found in Vincenti and Kruger [18].

Even though the governing equations take into account any number of monoatomic or diatomic species, the results shown correspond to a system of two chemical species:  $N_2$  and  $N$ . The relevant reactions are dissociations of  $N_2$  with  $N$  or  $N_2$  as catalysers.



Equations governing the evolution of the concentration  $X_1$  of  $N$  and  $X_2$  of  $N_2$ , starting from a given initial state ( $X_1^0, X_2^0$ ), are obtained by introducing the equilibrium constant  $K$  from (20) and (21).

$$\frac{dX_1}{dt} = 2(k_1 X_1 + k_2 X_2)(K X_2 - X_1^2) \quad (24)$$

$$X_1^0 + 2X_2^0 = C = X_1 + 2X_2 \quad (25)$$

If a time step  $\Delta t$  is used for the governing equations (1)-(4), the integration of (22) and (23) will give the concentrations  $X_1(\Delta t)$  and  $X_2(\Delta t)$  after  $\Delta t$ . Therefore, the source terms are

$$\dot{X}_i^{\text{react}} \Delta t = X_i(\Delta t) - X_i^0, \quad i = 1, 2 \quad (26)$$

The constants  $k_1$ ,  $k_2$ , and  $K$  are dependent on temperature  $T$ , and are obtained from Rakich, Bailey, and Park [19].

$$k_i(T) = a_i T^{s_i} \exp(-\frac{T_d^i}{T}), \quad i = 1, 2 \quad (27)$$

$$K = (A_1 + A_2 T + A_3 T^2) \exp(-\frac{T_d}{T}) \quad (28)$$

As a first approximation, we chose to consider isothermal reactions.

In the most general case with a large number of species the system of ordinary differential equations obtained for the evaluation of the concentration needs to be solved numerically. Moreover, its stiffness makes it necessary to use appropriate solvers such as DGEAR [20] from the IMSL library or the one proposed by Radhakrishnan [21]. But in the case of two species, the system can be integrated exactly as detailed below.

Substituting 21 into 20, one obtains

$$\frac{dX_1}{dt} = -2 \left( k_1 - \frac{k_2}{2} \right) X_1 + k_2 \frac{C}{2}$$

$$\left( X_1^2 + K \frac{X_1}{2} - \frac{KC}{2} \right) \quad (29)$$

Let us introduce  $\Delta = \frac{K^2}{4} + 2KC$ ,  $b = \frac{K/2 + \sqrt{\Delta}}{2}$ ,

$$d = \frac{K/2 - \sqrt{\Delta}}{2} - X_1^{eq}$$

Then if  $2k_1 \neq k_2$  the solution  $X_1$  obeys

$$f(X_1) = f(X_1^0) e^{-\frac{k_2}{a}(t-t_0)} \quad (30)$$

where  $a = \frac{k_2}{2k_1 - k_2}$  and

$$f(X_1) = \left| X_1 + a \right|^{(a-b)(a-d)} \left| X_1 + b \right|^{(b-a)(b-d)} X_1$$

$$+ \left| d \right|^{(d-a)(d-b)} \quad (31)$$

If  $2k_1 = k_2$  the the solution  $X_1$  must obey

$$g(X_1) = g(X_1^0) e^{-k_2 C (t-t_0)} \quad (32)$$

where  $g(X_1) = \left| (X_1+b)(X_1+d) \right|^{(d-b)}$  (33)

In both cases  $X_1$  is given by an implicit relation. These relations are easily solved in a few Newton's iterations, with a high precision. Moreover, an adequate change of variable can dramatically improve the convergence rate of the method.

Introducing

$$\alpha = \frac{X_1^0 - X_1^{eq}}{X_1 - X_1^{eq}} \quad (34)$$

where the superscript eq refers to equilibrium value of  $X_1$ , we can define  $\log(f(x)) = \phi(\alpha)$

Then  $X_1 = X_1^{eq} + \frac{X_1^0 - X_1^{eq}}{\alpha}$  and (35)

$$\phi(\alpha) = (a-b)(a-d) \log \left| (X_1^{eq} + a) + \frac{X_1^0 - X_1^{eq}}{\alpha} \right|$$

$$+ (b-a)(b-d) \log \left| X_1^{eq} + b + \frac{X_1^0 - X_1^{eq}}{\alpha} \right|$$

$$+ (d-a)(d-b) \log \left| \frac{X_1^0 - X_1^{eq}}{\alpha} \right| \quad (36)$$

We want to find  $\alpha$  such that

$$\phi(\alpha) = -\frac{k_2}{a}(t-t_0) \quad (37)$$

$\phi(\alpha)$  can be also considered as a function  $\Psi(u)$  of  $u = \log \alpha$ . We have to find  $\alpha = e^u$ , verifying that

$$\phi(\alpha) = \Psi(u) = -\frac{k_2}{a}(t-t_0) \quad (38)$$

We can apply Newton's method to find  $u$  (or  $\alpha$ )

$$\kappa(\alpha) = \frac{\partial \Psi}{\partial u} = \frac{(a-b)(a-d)}{1 + \alpha \left( \frac{X_1^{eq} + a}{X_1 - X_1^{eq}} \right)} + \frac{(b-a)(b-d)}{1 + \alpha \left( \frac{X_1^{eq} + b}{X_1 - X_1^{eq}} \right)}$$

$$+ (d-a)(d-b) \quad (39)$$

We want to solve  $\phi(d) = \Psi(u) = -\frac{k_2}{a}(t-t_0) = h$  (40)

Newton's method, applied to  $u$ , yields an iteration of the type

$$u^{n+1} = u^n + \frac{h - \Psi(u)}{\frac{\partial \Psi}{\partial u}} \quad (41)$$

Thus

$$\alpha^{n+1} = \alpha^n \exp \left( \frac{h - \phi(\alpha)}{\kappa(\alpha)} \right) \quad (42)$$

Such an iteration converges considerably faster than the primitive Newton method applied to  $X_1$ .

The same principle could be applied to the case of adiabatic reactions instead of isothermal reactions as assumed here.

Since Mac Cormack scheme is used to solve the governing equations, the source terms  $\dot{X}_{i,react}$  are evaluated at predictor step and also at corrector step, using the updated values of temperature.

#### NUMERICAL METHODS

The system of governing equations can be put into the form

$$\frac{\partial \vec{f}}{\partial t} = -\text{div}(\vec{F}(\vec{f})) + \vec{S} \quad (43)$$

where  $f$  is a vector whose  $n$  components are the unknowns  $\rho$ ,  $\rho u$ ,  $\rho e_t$ ,  $X_i$  the chemical composition and  $E_{vib}$  the vibrational energy.

$S$  is a vector containing the  $n$  source terms for the components of  $f$ .  $F$  is a function of  $f$  producing a matrix  $(n,2)$  in the 2D case, corresponding to the flux terms.

To integrate the differential system (1), our scheme is a modification of the classical two step explicit method of Mac Cormack [15].

These classical two steps are replaced in our computer code by three steps. The first two steps are strictly symmetrical, and thus allow use of the same subroutine to evaluate the new value at predictor and corrector steps. The last step is an averaging step:

$$\vec{f}_p^{n+1} = \vec{f}_p^n - (\overline{\text{DIV}}_F^+ (\vec{F} (\vec{f}_p^n)) - \vec{S}_p^n) \Delta t \quad (44)$$

$$\vec{f}_c^{n+1} = \vec{f}_p^{n+1} (\overline{\text{DIV}}_B^+ (\vec{F} (\vec{f}_p^{n+1})) - \vec{S}_p^{n+1}) \Delta t \quad (45)$$

$$\vec{f}^{n+1} = \frac{1}{2} (\vec{f}_p^n + \vec{f}_c^{n+1}) \quad (46)$$

$\text{DIV}_F^+$  and  $\text{DIV}_B^+$  represent forward and backward discretization of the operator divergence, subscript  $p$  refers to predicted values, superscript  $n$  indicates the time step at which the values are evaluated.

To increase the versatility of the code, a zonal approach similar to the one used by Veuillot and Meauze [22], has been introduced. The computational domain  $D$  can be decomposed into subdomains  $D_1, D_2, \dots, D_m$ . In each of the subdomains, different densities of grid points can be used.

To allow an easy definition of complex shapes and boundaries, an indirect addressing technique is used (fig. 1).

Two integer arrays store the indices  $i_{bo}(n, i_b)$ ,  $j_{bo}(n, i_b)$  of the  $n$ -th point of the boundary  $i_b$ . The artificial boundaries (connection between two domains) are defined in the same manner.

This technique can easily be extended to three dimensional codes (fig.1). It allows the use of code for internal as well as external flows with very simple changes in the set of input data.

At the present time, eight types of boundaries have been introduced in the code. They are: inlet, isothermal wall, adiabatic wall, exit, secondary inlet (to simulate injection of chemical species in the field), connection between domains, far field, and symmetry.

#### ARTIFICIAL DISSIPATION

To improve the numerical stability of the code and to allow its application to very strong shocks, the choice of an adequate artificial dissipation is crucial. Before implementing a more sophisticated dissipative concept, such as a TVD scheme [23], it is prudent to implement a simpler artificial viscosity that can be used afterwards as a reference. The extension of the Lapidus artificial viscosity [24] extended by Lohner et al. [25] to multidimensional problems, has been included in the code as follows. After each iteration,  $n$ , we correct the new values of

the variables in the field,  $Q_{ijk}^n$ , by applying:

$$Q_{i,j,k}^n = Q_{i,j,k}^n + \Delta t \sum_{i=1}^2 \frac{\partial}{\partial x^i} (k^{ij} \frac{\partial Q^n}{\partial x^j}) \quad (47)$$

where

$$k^{ij} = \ell^i k \ell^j, \quad (48)$$

and

$$\ell = (\ell^2)^{1/2} = \frac{\nabla |u|}{|\nabla |u|} \quad (49)$$

is pointing in the direction of maximum change of magnitude of flow velocity vector  $u$ . The parameter  $k$  is given by:

$$k = C_k h^2 \left| \frac{\partial u \cdot \ell}{\partial \ell} \right| \quad (50)$$

where  $h$  is a representative grid size and  $C_k$  is an arbitrary constant (typically equal to 1 or 2). In the program, this constant can be different for each variable, even equal to zero if no artificial dissipation is desired for a given variable.

Such an artificial viscosity has been chosen for its ease of implementation, and because it vanishes in a viscous boundary layer, where an artificial viscosity is undesirable.

#### RESULTS

Before running the code, it is necessary to assess the validity of the chemical kinetics solver. Therefore, the subroutine used to predict the evolution of species concentration, with Newton's iteration technique, has been tested separately. These results have been compared with the theoretical curves obtained by plotting the concentration versus the evolution of time which is given explicitly by equation (31). This test has been done for the dissociation of  $O_2$  (fig. 2) and the dissociation of  $N_2$  (fig. 3). In both cases the solver proved to be accurate and very fast.

Then, the complete hypersonic flow analysis code was applied to three different test cases. For all three cases, the geometry is a rectangular box (fig. 4), closed, filled with a mixture of molecular nitrogen,  $N_2$ , and with atomic nitrogen,  $N$ .

For the first test case, the box is at a given uniform temperature  $T$  and pressure  $P$ . Nevertheless, the initial concentrations of  $N_2$  and  $N$  do not correspond to equilibrium composition for the initial pressure and temperature. A very small time step is therefore chosen, adapted to the chemical reactions ( $\Delta t = 1E-18$  sec). The mixture temperature and pressure increase and in turn the equilibrium composition is modified. A steady equilibrium is finally reached as shown by the plot of pressure versus time at a point near the vertical walls (fig. 5). The recombination of  $N$  yield a final pressure and temperature higher than their initial values.

In the second test case, the box is initially partitioned by a membrane. The pressures and temperatures on the two sides of

the box are the same and the compositions are different. For this test case, we freeze the chemical reactions, that is, we impose a species production term always equal to zero. In this situation, the possible physical phenomena are limited to diffusion and convection only. These processes are considerably slower than the chemical reactions as the flow is nearly motionless. Therefore, a much larger total time interval is needed to reach the equilibrium. As expected, the concentrations of  $N_2$  and  $N$  tend to become uniform in the box (fig. 6) and the pressure returns to its initial value.

The third test case differs from the second case only by taking into account the equilibrium chemistry. The diffusion of mass, momentum and energy is a relatively slow process. The convective terms also appear. Thus, the main effect is due to the chemical reactions. The initial condition corresponds to a mixture with a concentration of  $N$  that is higher than the equilibrium value for the local pressure and temperature. Thus, the atoms of  $N$  will tend to recombine, as in the first test case. At  $t=0$ , pressure and temperature are the same on both sides of the membrane. But, the density and the molar masses are different since they correspond to different equilibrium compositions. In turn, the heat released by the chemical reactions on the two sides of the membrane will be different for  $t > 0$ . Therefore, strong gradients of pressure and temperature appear. As a result, an acoustic wave develops and propagates into the box [6], as shown in fig. 7. The frequency of this wave corresponds clearly to the first longitudinal mode of excitation of the box. A strong damping of the wave can also be observed in the fig. 7. The last part of the curve corresponds to convection and diffusion processes, tending to produce a uniform temperature and composition. This computation is performed with quite a large time step ( $\Delta t = 2E-7$  sec). One thousand iterations, for 110 grid points took 8 minutes on a VAX 8550. It should be pointed out that even though this test case corresponds to equilibrium chemistry, we let the complete hypersonic flow analysis computer program compute the source terms as the limit of nonequilibrium chemistry source terms.

#### ACKNOWLEDGEMENTS

This research has been supported by NASA Ames Grant NCA 2-120 and by Direction des Recherches, Etudes et Techniques under contract 85.34.1385 while Mr. Lionel Marraffa was a Visiting Research Scientist at the Penn State University. Special thanks are due to Ms. Amy Myers for her superb typing and to Dr. Chul Park and other colleagues at NASA Ames Research Center for their valuable discussions.

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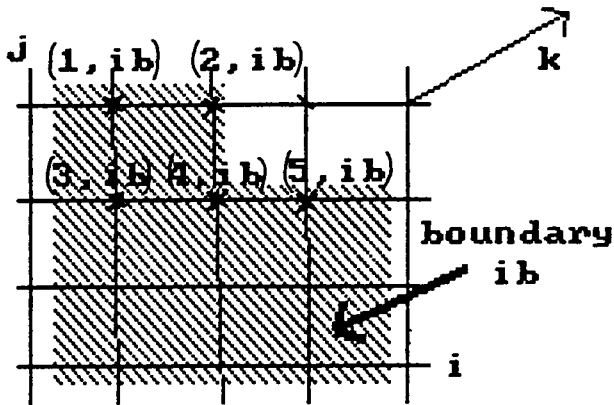


FIGURE 1: GEOMETRICAL DEFINITION OF BOUNDARIES

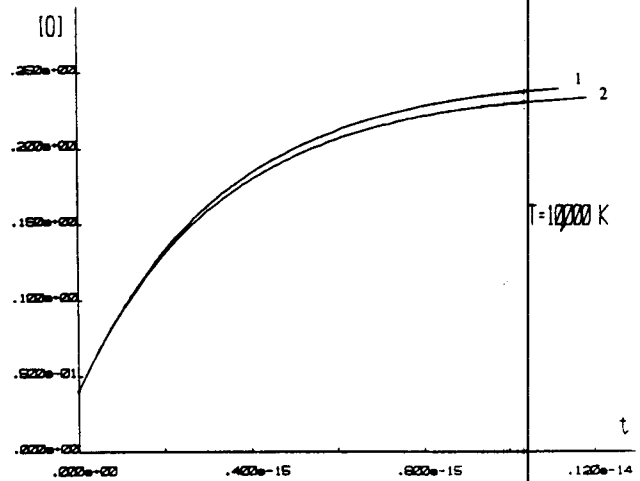


fig.2: VALIDATION OF THE ODE SOLVER: CASE OF [C]  
1: THEORY ; 2: NEWTON'S ITERATION

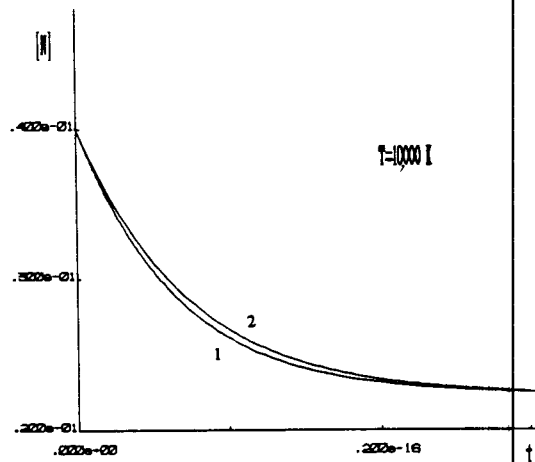


fig.3: VALIDATION OF THE ODE SOLVER: CASE OF [N]  
1: THEORY 2: NEWTON'S ITERATION

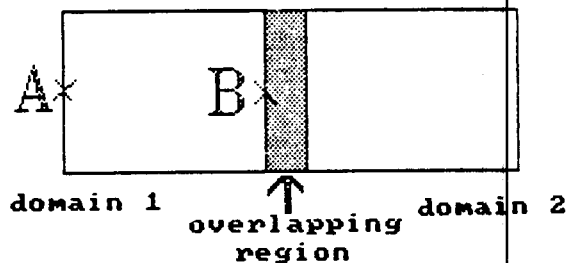


fig.4: TEST CASE GEOMETRY



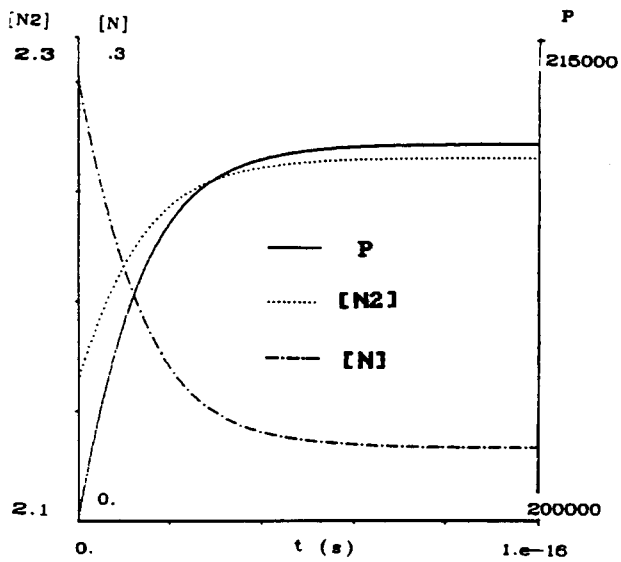


fig.5: VARIATION OF PRESSURE AND CONCENTRATION OF  $[N]$  VERSUS TIME ( REACTING MIXTURE ) ( UNIFORM INITIAL COMPOSITION )

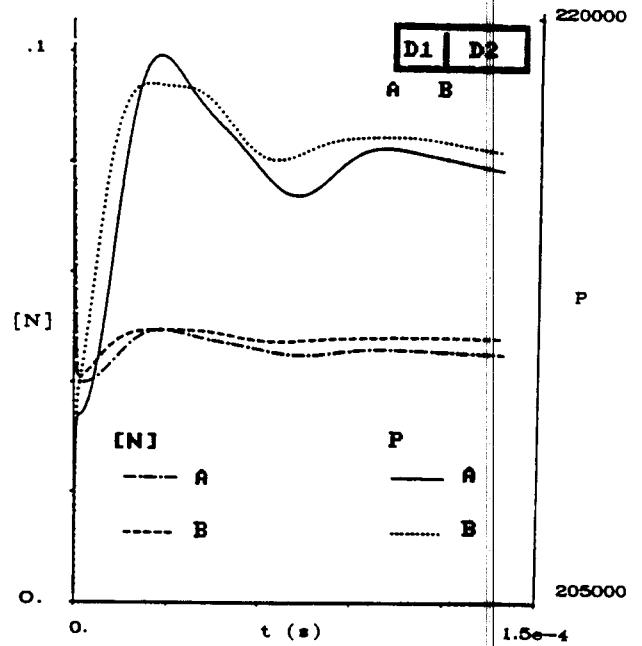


fig.7: VARIATION OF PRESSURE AND CONCENTRATION OF N VERSUS TIME ( REACTING MIXTURE ) ( NONUNIFORM INITIAL COMPOSITION )

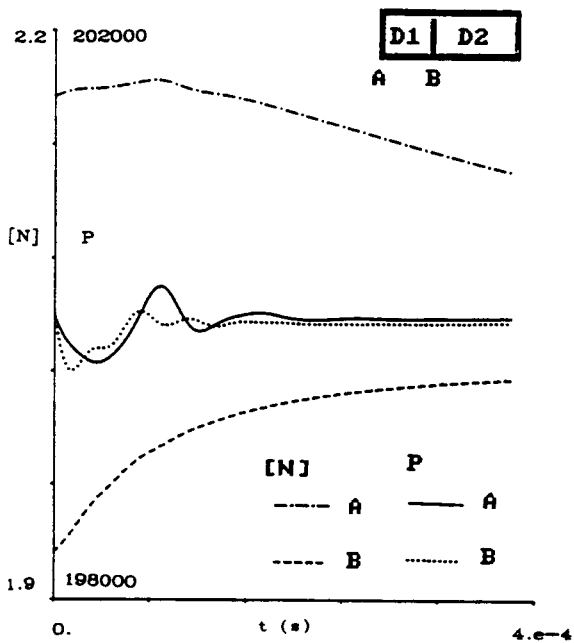


fig.8: VARIATION OF PRESSURE AND CONCENTRATION OF N VERSUS TIME ( NONUNIFORM INITIAL COMPOSITION )