AXISYMMETRIC TWO-PHASE REACTING GAS NONEQUILIBRIUM NOZZLE FLOWS ANALYSIS

02274-6007-R000

18 AUGUST 1967

Prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

MANNED SPACECRAFT CENTER

UNDER CONTRACT NAS 9-4358

TRW SYSTEMS GROUP

One Space Park, Redondo Beach, California

AXISYMMETRIC TWO-PHASE REACTING GAS NONEQUILIBRIUM NOZZLE FLOWS ANALYSIS

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FOREWORD

The three parts of a computer program based on the analysis given in this report have been programmed for use on an IBM 7094 computer. The one-dimensional two-phase reacting gas part was programmed by H. M. Frey. The axisymmetric two-phase transonic part was programmed by J. E. Melde. The axisymmetric two-phase characteristics part was programmed by G. R. Nickerson and J. E. Melde. These three parts have not been combined into a functioning program, however, since the size of the resulting program necessitates an excessive number of overlays during program execution causing extremely long running time per case (greater than one hour) on an IBM 7094 computer.

CONTENTS

NOMENCLATURE

a	Reaction rate parameter
A	Function defined by Equation (2-44)
b	Reaction rate parameter
B	Function defined by Equation (2-45)
c	Specifies mass fraction
C	Function defined by Equation (2-46)
C_{Di}	Particle drag coefficient
C_p	Heat capacity of gas phase at constant pressure
C_{ppi}	Heat capacity of particle at constant pressure
D	Function defined by Equation (2-47)
E	Function defined by Equation (2-48)
f	Derivative
f_{pi}	Drag coefficient ratio, $C_{Di}/(C_{Di})_{stokes}$
F	Free energy, also function defined by Equation (2-38)
g_{pi}	Heat transfer coefficient ratio, $Nu_i/(Nu_i)_{stokes}$
G	Function defined by Equation (2-39)
h	Enthalpy, also integration increment
H	Total enthalpy, also function defined by Equation (2-40)
ΔH_{pi}	Latent heat of melting
k	Variable increment, also reaction rate parameter
K	Equilibrium constant
K_{pi}	Function defined by Equation (2-43)

NOMENCLATURE (Continued)

m	Reaction rate ratio
m_{pi}	Particle bulk density
M	Mach number, also third body reaction term
n	Reaction rate parameter
Nu_i	Particle Nusselt number
P	Pressure
Pr	Gas Prandtl number
r	Radial distance
r_{pi}	Particle radius
r^*	Nozzle throat radius
R	Gas Constant
R^*	Nozzle wall radius of curvature at throat
T	Temperature
T_{pmi}	Melting temperature
u	Velocity in x-direction
v	Velocity in r-direction
V	Flow velocity
x	Axial distance
y	Dependent variable
z	Dependent variable
$\beta_{i,j}$	Partial derivative
$\emptyset_{i,j}$	Partial derivative

NOMENCLATURE (Continued)

γ	Gamma
ψ	Particle stream function
ρ	Density
ρ_{pi}	Particle density in gas phase
μ	Gas viscosity
θ	Flow angle
ω	Species mass production rate

Subscripts:

i	Refers to ith species or equation
j	Refers to jth reaction or variable
pi	Refers to ith particle size group

Superscripts:

*	Refers to throat conditions or sonic conditions

1. INTRODUCTION

This report contains an analysis of two-phase reacting gas nonequilibrium flows in axisymmetric nozzles. This study was performed by TRW Systems for NASA(MSC) under Contract NAS9-4358, Improvement of Analytical Predictions of Delivered Specific Impulse.

The objective of this contract was to develop a family of four computer programs to calculate inviscid, one-dimensional and axisymmetric nonequilibrium nozzle flow fields accounting for the nonequilibrium effects of finite rate chemical reactions between gaseous combustion products and velocity and thermal lags between gaseous and condensed combustion products.

The four programs developed under this contract are:

- A one-dimensional program which calculates the equilibrium, frozen and kinetic performance of propellant systems having gaseous exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine.

- A one-dimensional program which calculates the equilibrium frozen and kinetic performance of systems having gaseous and condensed exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine, chlorine and one metal element, either aluminum, beryllium, boron or lithium.

- An axisymmetric program which calculates the kinetic performance of propellant systems having gaseous exhaust products containing the elements carbon, hydrogen, oxygen, nitrogen, fluorine, and chlorine. On option, this program considers either the expansion of a uniform mixture (the ideal engine case) or a two-zone mixture (the film cooled engine case).

- A Fortran IV version of an axisymmetric program which calculates the performance of propellant systems having both gaseous and condensed exhaust

products. This program considers only the expansion of a uniform mixture (the ideal engine case).

The first three programs differ in a number of ways from previous programs developed to calculate nonequilibrium nozzle expansions. In particular:

- The programs are completely self-contained requiring specification of only the propellant system (elemental composition and heat of formation), relaxation rates and nozzle geometry to run a case.

- The chemical species considered by the programs have been selected to allow accurate equilibrium, frozen and kinetic performance analyses of cryogenic, space storable, pre-packaged, hybrid, and solid propellant systems of current and projected operational use.

- All dissociation-recombination and binary exchange reactions between the gaseous species present in the exhaust are considered by the programs allowing complete kinetic expansion calculations.

- The programs utilize TRW Systems implicit integration method which allows rapid integration of the chemical and gas-particle relaxation equations from equilibrium chamber conditions.

- The programs allow analysis of the performance loss associated with film cooling in propellant systems having all gaseous exhaust products.

- The programs allow simultaneous consideration of both chemical and gas-particle relaxation losses in propellant systems having condensed exhaust products.

- The one-dimensional programs allow equilibrium, frozen and kinetic performance calculations to be performed during a single machine run.

- The programs are written in machine independent language (Fortran IV) allowing their use on all standard computers.

The fourth program utilizes standard explicit integration methods. This program is an undated Fortran IV version of an earlier program which allows the determination of the performance losses associated with velocity and thermal lags between gaseous and condensed combustion products in axisymmetric nozzles, but does not account for the nonequilibrium effects of finite rate chemical reactions between gaseous combustion products.

The study described in this report was performed to initiate the development of an additional computer program to calculate the performance of propellant systems in axisymmetric nozzles accounting for the nonequilibrium effects of both finite rate chemical reactions between gaseous combustion products and velocity and thermal lags between gaseous and condensed combustion products. This report contains a description of the equations governing the flow field and of the method of numerical solution. The assumptions made in the analysis and the method of integrating the governing equations are parallel to those of the first three programs developed. The computer program consists of three major parts: the one-dimensional two-phase reacting gas part which is the One-Dimensional Two-Phase Reacting Gas Nonequilibrium Performance Program, the axisymmetric two-phase transonic part, and the axisymmetric two-phase characteristics part. These parts have been programmed, but have not been combined into a functioning program since the large size of the complete program necessitates an excessive number of overlays during program execution causing extremely long computer time per case (greater than one hour).

A program based on the present effort may be put into operational form when larger computers (greater than 32K cores) become available. Upon completion, this program will calculate

the inviscid axisymmetric nonequilibrium nozzle expansion of propellant exhaust mixtures co ·ıining the six elements: carbon, hydrogen, oxygen, nitrogen, fluorine, and chlorine and one metal element, either aluminum, beryllium, boron or lithuim. The computer program will consider all significant gaseous species present in the exhaust mixtures of propellants containing these elements and all gas phase chemical reactions which can occur between the exhaust products. The program will also consider the velocity and thermal lags (for five particle groups) between the gaseous and condensed combustion products (when they are present in the chamber). The program will not consider mass transfer (only momentum and energy transfer) between gaseous and condensed combustion products. The program will calculate only the expansion of uniform mixtures (the ideal engine case).

In the program, the initial data line required to start the characteristic calculations is obtained from an appropriate transonic analysis which utilizes the results of the one-dimensional two-phase reacting gas program. The characteristic equations governing the fluid dynamic variables are integrated using a second order (modified Euler) explicit integration method while the chemical and particle relaxation equations are integrated using a first order implicit integration method to insure numerical stability in near equilibrium flows.

Section 2 contains a derivation of the equations governing the inviscid axisymmetric flow of a two-phase reacting gas mixture in the form in which they are integrated in the computer program and a description of the method used to calculate the transonic initial line which is used to start the characteristic calculations.

Section 3 contains a description of the integration methods used to calculate the fluid dynamic variables, the chemical species, and the particle properties.

Section 4 contains a discussion of developing a computer program based on the present analysis.

2. ANALYSIS

2.1 CONSERVATION EQUATIONS

The conservation equations governing the inviscid axisymmetric flow of a two phase reacting gas mixture can be simply derived utilizing the following assumptions:

- There are no mass or energy losses from the system
- The gas is inviscid except for its interactions with the condensed particles
- Each component of the gas is a perfect gas
- The internal degrees of freedom (rotational and vibrational) of each component of the gas are in equilibrium
- The volume occupied by the condensed particles is negligible
- The thermal (Brownian) motion of the condensed particles is negligible
- The condensed particles do not interact
- The condensed particle size distribution may be approximated by groups of different size spheres
- The internal temperature of the condensed particles is uniform
- Energy exchange between the gas and the condensed particles occurs only in convection
- The only forces on the condensed particles are viscous drag forces
- There is no mass transfer from the gas to the condensed phase during the nozzle expansion

These assumptions have been previously used in all studies of reacting gas[1] and gas-particle[2] nozzle flows.

The conservation equations are derived here in the form used in the present analysis.

For each component of the gas the continuity equation is

$$(\rho_i u)_x + \frac{1}{r}(r\rho_i v)_r = \omega_i r^* \qquad (2\text{-}1)$$

where the axial coordinates (r, x) have been normalized with the throat radius. Summing over all components of the mixture, the overall continuity equation for the gas is obtained

$$(\rho u)_x + \frac{1}{r}(r\rho v)_r = 0 \qquad (2\text{-}2)$$

By use of the above equation, Equation (2-1) can be rewritten as

$$u(c_i)_x + v(c_i)_r = \frac{\omega_i r^*}{\rho} \qquad (2\text{-}3)$$

For each particle size group the continuity equation is

$$(\rho_{pi}\, u_{pi})_x + \frac{1}{r}(r\rho_{pi}\, v_{pi})_r = 0 \qquad (2\text{-}4)$$

since there is no mass transfer from the gas to the condensed phase.

The overall momentum equations for the mixture are

$$\rho(uu_x + vu_r) + \sum_{i=1} \rho_{pi}\left[u_{pi}(u_{pi})_x + v_{pi}(u_{pi})_r\right] + P_x = 0 \qquad (2\text{-}5)$$

$$\rho(uv_x + vv_r) + \sum_{i=1} \rho_{pi}\left[u_{pi}(v_{pi})_x + v_{pi}(v_{pi})_r\right] + P_r = 0 \qquad (2\text{-}6)$$

The overall energy equation for the mixture is

$$\rho\left[uh_x + vh_r + u(uu_x + vu_r) + v(uv_x + vv_r)\right]$$

$$+ \sum_{i=1} \rho_{pi}\Big\{ u_{pi}(h_{pi})_x + v_{pi}(h_{pi})_r + u_{pi}\left[u_{pi}(u_{pi})_x + v_{pi}(u_{pi})_r\right]$$

$$+ v_{pi}\left[u_{pi}(v_{pi})_x + v_{pi}(v_{pi})_r\right]\Big\} = 0 \qquad (2\text{-}7)$$

where for the gas phase

$$h = \sum_{i=0} c_i h_i \qquad (2\text{-}8)$$

and

$$h_i = \int_o^T C_{pi}\,dT + h_{io} \qquad (2\text{-}9)$$

while for each particle group

$$h_{pi} = \int_o^{T_{pi}} C_{ppi}\,dT + h_{io} \quad , \; T_{pi} < T_{pmi} \qquad (2\text{-}10)$$

and

$$h_{pi} = \int_o^{T_{pi}} C_{ppi}\,dT + h_{io} + \Delta H_{pi}, \; T_{pi} > T_{pmi} \qquad (2\text{-}11)$$

For each component of the gas, the equation of state is

$$P_i = \rho_i R_i T \qquad (2\text{-}12)$$

Summing over all components of the mixture, the overall equation of state for the gas is obtained

$$P = \rho R T \qquad (2\text{-}13)$$

where

$$R = \sum_{i=1} c_i R_j \qquad (2\text{-}14)$$

The particle drag equations are

$$u_{pi}(u_{pi})_x + v_{pi}(u_{pi})_r = \frac{9}{2}\frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2}(u - u_{pi}) \qquad (2\text{-}15)$$

$$u_{pi}(v_{pi})_x + v_{pi}(v_{pi})_r = \frac{9}{2}\frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2}(v - v_{pi}) \qquad (2\text{-}16)$$

and the particle heat transfer equation is

$$u_{pi}(h_{pi})_x + v_{pi}(h_{pi})_r = -\frac{3\,\mu g_{pi} r^*}{m_{pi} r_{pi}^2}\frac{C_p}{Pr}(T_{pi} - T) \qquad (2\text{-}17)$$

By standard methods,[3] the characteristic relationships for the conservation equations can be shown to be

$$\frac{dr}{dx} = \tan\theta \qquad (2\text{-}18)$$

$$d\frac{V^2}{2} + \frac{dP}{\rho} = \frac{C}{\cos\theta}\,dx \qquad (2\text{-}19)$$

$$\frac{dP}{\gamma P} - \frac{d\rho}{\rho} = \frac{A}{\cos\theta}\,dx \qquad (2\text{-}20)$$

$$\frac{\gamma-1}{\gamma}\frac{dP}{P} - \frac{dT}{T} = \frac{B}{\cos\theta}\,dx \qquad (2\text{-}21)$$

$$dc_i = \frac{\omega_i r^*}{\rho V\cos\theta}\,dx \qquad (2\text{-}22)$$

along streamlines,

$$\frac{dx}{dr} = \cot(\theta + \alpha) \qquad (2\text{-}23)$$

$$\frac{dP}{P} = G\left[\left(D - \frac{\sin\theta}{r}\right)F\,dr - d\theta\right] \qquad (2\text{-}24)$$

along left running characteristics,

$$\frac{dr}{dx} = \tan(\theta - \alpha) \tag{2-25}$$

$$\frac{dP}{P} = -G\left(E - \frac{\sin\theta}{r}\right) H\, dx - d\theta \tag{2-26}$$

along right running characteristics,

$$\frac{dr_{pi}}{dx_{pi}} = \tan\theta_{pi} \tag{2-27}$$

$$u_{pi}\, du_{pi} = \frac{9}{2}\frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2}(V\cos\theta - u_{pi})\, dx_{pi} \tag{2-28}$$

$$v_{pi}\, dv_{pi} = \frac{9}{2}\frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2}(V\sin\theta - v_{pi})\, dr_{pi} \tag{2-29}$$

$$u_{pi}\, dh_{pi} = -\frac{3\mu g_{pi} r^*}{m_{pi} r_{pi}^2}\frac{Cp}{Pr}(T_{pi} - T)\, dx_{pi} \tag{2-30}$$

$$d\psi_{pi} = 0 \tag{2-31}$$

along particle streamlines, where

$$V = (u^2 + v^2)^{1/2} \tag{2-32}$$

$$\theta = \tan^{-1}\left(\frac{v}{u}\right) \tag{2-33}$$

$$\alpha = \sin^{-1}\left(\frac{1}{M}\right) \tag{2-34}$$

$$M = \frac{V}{(\gamma R T)^{1/2}} \tag{2-35}$$

$$\gamma = \frac{Cp}{C_p - R} \tag{2-36}$$

$$C_p = \sum_{i=1} c_i C_{pi} \tag{2-37}$$

$$F = \cos\theta - \sin\theta\cot(\theta+\alpha) \tag{2-38}$$

$$G = \frac{\gamma}{\sin\alpha\cos\alpha} \tag{2-39}$$

$$H = \cos\theta \tan(\theta - \alpha) - \sin\theta \tag{2-40}$$

$$V_{pi} = (u_{pi}^2 + v_{pi}^2)^{1/2} \tag{2-41}$$

$$\theta_{pi} = \tan^{-1}\left(\frac{v_{pi}}{u_{pi}}\right) \tag{2-42}$$

$$K_{pi} = V_{pi}\left(\cos\theta_{pi}\cos\theta + \sin\theta_{pi}\sin\theta\right) \tag{2-43}$$

$$A = \frac{r^*}{PV}\sum_{i=1}\omega_i R_i T - B \tag{2-44}$$

$$B = \frac{\gamma-1}{\gamma}\frac{r^*}{PV}\left\{\sum_{i=1}\omega_i h_i - \sum_{i=1}\rho_{pi}\left[\frac{9}{2}\frac{\mu f_{pi}}{m_{pi} r_{pi}^2}\left(V^2+V_{pi}^2-2VK_{pi}\right)\right.\right.$$
$$\left.\left.+\frac{3\mu g_{pi}}{m_{pi} r_{pi}^2}\frac{C_p}{Pr}\left(T_{pi}-T\right)\right]\right\} \tag{2-45}$$

$$C = -\frac{r^*}{\rho}\sum_{i=1}\rho_{pi}\frac{\mu f_{pi}}{m_{pi} r_{pi}^2}\left(V - K_{pi}\right) \tag{2-46}$$

$$D = A + \frac{r^*}{\rho V}\sum_{i=1}\rho_{pi}\frac{9}{2}\frac{\mu f_{pi}}{m_{pi} r_{pi}^2}\left\{1 - \frac{V_{pi}}{VF}\left[\cos\theta_{pi} - \sin\theta_{pi}\cot(\theta+\gamma)\right]\right\} \tag{2-47}$$

$$E = A + \frac{r^*}{\rho V}\sum_{i=1}\rho_{pi}\frac{9}{2}\frac{\mu f_{pi}}{m_{pi} r_{pi}^2}\left\{1 - \frac{V_{pi}}{VH}\left[\cos\theta_{pi}\tan(\theta-\gamma) - \sin\theta_{pi}\right]\right\} \tag{2-48}$$

The above form of the characteristic relationship remains determinate when the streamline is horizontal, when the left running characteristic is vertical, or when the right running characteristic is horizontal. Rarely (if ever) will the inverse of the three situations occur in nozzle flow field calculations.

The present program is written to calculate the nonequilibrium nozzle expansion of propellant exhaust mixtures containing the six elements: carbon, hydrogen, oxygen, nitrogen, fluorine and chlorine and one metal element, either aluminum, beryllium, boron or lithium. Gold[4] has established the species and chemical

reactions that need to be considered in calculating nozzle expansions of propellant exhaust mixtures containing these elements. These species and chemical reactions have been listed in Tables 2-1 through 2-7 of Reference 5. The net species production rate (ω_i) for each species considered by the program is calculated from

$$\omega_i = \bar{m}_i \rho^2 \sum_{j=1} (\nu'_{ij} - \nu_{ij}) X_j \qquad (2\text{-}49)$$

where the net production rate for each reaction (X_j) considered by the program is calculated from

$$X_j = \left[K_j \prod_{i=1} c_i^{\nu_{ij}} - \rho \prod_{i=1} c_i^{\nu'_{ij}} \right] M_j k_{Rj} \qquad (2\text{-}50)$$

for the dissociation-recombination reactions and

$$X_j = \left[K_j \prod_{i=1} c_i^{\nu_{ij}} - \prod_{i=1} c_i^{\nu'_{ij}} \right] k_{Rj} \qquad (2\text{-}51)$$

for the binary exchange reactions.

The stoichiometric coefficients appearing in the above equations (ν_{ij} and ν'_{ij}) are defined by the generalized chemical reaction equation

$$\sum_{i=1} \nu_{ij} \bar{M}_i \rightleftharpoons \sum_{i=1} \nu'_{ij} \bar{M}_i \qquad (2\text{-}52)$$

where $\bar{M}_i$ represents the ith chemical species.

Since each dissociation-recombination reaction has a distinct reaction rate associated with each third body, the net production rate for each dissociation-recombination reaction should be calculated from

$$X_j = \sum_{k=1} \left[K_j \prod_{i=1} c_i^{\nu_{ij}} - \rho \prod_{i=1} c_i^{\nu'_{ij}} \right] c_k \, k_{Rkj} \qquad (2\text{-}53)$$

rather than Equation (2-50). Benson and Fueno[6] have shown theoretically that the temperature dependence of recombination rates is approximately independent of the third body. Available experimental recombination rate data also indicate that the temperature dependence of recombination rate is independent of the third body within the experimental accuracy of the measurements. Assuming that the temperature dependence of recombination rates is independent of the third body, the recombination rate associated with the kth species (third body) can be represented as

$$k_{Rkj} = a_{kj} \, T^{-n_j} \, e^{-b_j/T} \qquad (2\text{-}54)$$

where only the constant a_{kj} is different for different species (third bodies). From Equation (2-53) it can be shown that

$$X_j = \left[K_j \prod_{i=1} c_i^{\nu_{ij}} - \rho \prod_{i=1} c_i^{\nu'_{ij}} \right] \sum_{k=1} a_{kj} \, c_k \, T^{-n_j} \, e^{-b_j/T}$$

$$= \left[K_j \prod_{i=1} c_i^{\nu_{ij}} - \rho \prod_{i=1} c_i^{\nu'_{ij}} \right] \left[\sum_{i=1} \frac{a_{ij}}{a_{kj}} \, c_i \right] a_{kj} \, T^{-n_j} \, e^{-b_j/T} \qquad (2\text{-}55)$$

Thus the recombination rates associated with each third body can be considered as in Equation (2-50) by calculating the general third body term (M_j) as

$$M_j = \sum_{i=1} m_{j,i} \, c_i \qquad (2\text{-}56)$$

where $m_{j,i}$ is the ratio $\frac{a_{ij}}{a_{kj}}$ of the recombination rate associated with the ith species (third body) to the recombination rate associated with the kth species (third body) which is the reference species (third body) whose rate [in the form of Equation (2-54)] is specified in the program input.

2.2 INITIAL LINE CONSTRUCTION

In principle, one can solve the proceeding equations using perturbation methods to obtain asympotic expansions for the subsonic and transonic flow fields as has been done for nonreacting gas flows.[7] Such solutions are extremely complex for nonequilibrium flows however, and it is doubtful if more than one term of the expansion can be determined.

An alternate method of constructing nonequilibrium initial lines for characteristic calculations is to determine the effect of nozzle curvature on the gas flow field using an average expansion coefficient to approximate the nonequilibrium expansion process through the throat region and to then calculate the effect of the altered gas flow field on the relaxation processes. This method (which is the equivalent to the first step of a relaxation process) has been successfully used by Kliegel and Nickerson[8] in two-phase flow nozzle studies to predict nozzle inlet angle and throat curvature effects. It was chosen for use in this program because of its relative simplicity and proven accuracy. The calculations performed in constructing the nonequilibrium initial lines used as starting lines for the characteristic calculations are summarized below.

2.2.1 Gas Flow Field

A one dimensional calculation is performed from the chamber to the throat for the propellant system and nozzle geometry of

interest using the One-Dimensional Two-Phase Reacting Gas Nonequilibrium Performance Program[5] and tables of flow properties (ϱ, V, T), species concentrations (c_i) and particle properties (V_{pi}, T_{pi}) are constructed as a function of pressure starting at the throat.

An average expansion coefficient in the throat region is calculated from

$$\bar{\gamma} = \frac{\ln (P_{20}/P_1)}{\ln (\rho_{20}/\rho_1)} \qquad (2\text{-}57)$$

where the subscripts 1 and 20 refer to the first and last table entries.

An axisymmetric uniform expansion transonic flow field is constructed for the nozzle of interest using this average expansion coefficient and the second order analysis of Kliegel and Quan.[7]

The pressure, location and gas flow angle variation along the constant pressure line originating at a specified wall point are determined.

The remaining gas flow properties (ϱ, V, T) and species concentrations (c_i) along the constant pressure line are determined by interpolation on pressure from the tables previously constructed with the One-Dimensional Two-Phase Reacting Gas Nonequilibrium Performance Program.

2.2.2 Particle Flow Field

The particle flow angle variation along the above constant pressure line is calculated from the constant fraction lag relationship

$$\frac{du}{dx}\left(\frac{dv}{dx}\right)^{-1}\left[\frac{\sqrt{1+\frac{8}{9}\frac{m_{pi}r_{pi}^2}{u f_{pi} r^*}\cot\theta_{pi}\frac{dv}{dx}}-1}{\sqrt{1+\frac{\varepsilon}{9}\frac{m_{pi}r_{pi}^2}{u f_{pi} r^*}\frac{du}{dx}}-1}\right] \quad \tan\theta = 1 \qquad (2\text{-}28)$$

where $\frac{du}{dx}$ and $\frac{dv}{dx}$ are the gas velocity derivatives along the particle streamlines. These derivatives are calculated from

$$\frac{du}{dx} = V^* \left\{ \frac{1}{\sqrt{R}} \left[\frac{da_o}{dz} + \frac{1}{R} \left(\frac{db_o}{dz} + \frac{db_2}{dz} r^2 \right) + \frac{1}{R^2} \left(\frac{dc_o}{dz} + \frac{dc_2}{dz} r^2 + \frac{dc_4}{dz} r^4 \right) \right] + \frac{1}{R} \left[2b_2 r + \frac{1}{R} \left(2c_2 r + 4c_4 r^3 \right) \right] \tan\theta_{pi} \right\} \quad (2\text{-}59)$$

$$\frac{dv}{dx} = V^* \left\{ \frac{1}{R} \left[\frac{da_1}{dz} r + \frac{1}{R} \left(\frac{db_1}{dz} r + \frac{db_3}{dz} r^3 \right) + \frac{1}{R^2} \left(\frac{dc_1}{dz} r + \frac{dc_3}{dz} r^3 + \frac{dc_5}{dz} r^5 \right) \right] + \frac{1}{\sqrt{R}} \left[a_1 + \frac{1}{R} (b_1 + 3b_3 r^2) + \frac{1}{R^2} (c_1 + 3c_3 r^2 + 5c_5 r^4) \right] \right\} \tan\theta_{pi} \quad (2\text{-}60)$$

where the coefficients a_i, b_i, and c_i are those derived by Kliegel and Quan.[7]

The particle velocities and temperature along the constant pressure line are calculated from

$$u_{pi} = V_{pi}(0) \cos\theta_{pi} \quad (2\text{-}61)$$

$$v_{pi} = V_{pi}(0) \sin\theta_{pi} \quad (2\text{-}62)$$

$$T_{pi} = T_{pi}(0) \quad (2\text{-}63)$$

where the values on the initial line axis $\left[V_{pi}(0) \text{ and } T_{pi}(0) \right]$ are determined by interpolation on pressure from the tables previously constructed with the One-Dimensional Two-Phase Reacting Gas Nonequilibrium Performance Program.

The axis particle density $\rho_{pi}(0)$ is evaluated by integrating the particle continuity and drag equations along the axis using Kliegel and Quan's[7] second order analysis for the gas velocity and relating the axial particle velocity to the gas axial velocity through the constant fractional lag relationships. The particle densities along the constant pressure line are then calculated from

$$\rho_{pi} = \rho_{pi}(0) \tag{2-64}$$

The constant pressure line is then integrated to determine the gas mass flow $\dot{m}$ where

$$\dot{m} = 2\pi \int_{axis}^{wall} r\rho V(\cos\theta dr - \sin\theta dx) \tag{2-65}$$

and the particle limiting streamline location is determined from the particle continuity relationship across the initial line

$$\dot{m}\, W_{pi} = 2\pi \int_{axis}^{\text{limiting streamline}} r\, \rho_{pi}(u_{pi}dr - v_{pi}dx) \tag{2-66}$$

where W_{pi} is particle to gas mass flow ratio for the ith particle size group.

2.2.3 Discussion of Initial Line Results

The above method of constructing initial lines for nonequilibrium characteristic calculations accounts for the dominant curvature effects on the gas and particle flow fields through second order and ignores the curvature effects which would cause a constant pressure line, chosen as the initial starting line, not to be a constant property line. By comparing the above method of constructing nonequilibrium initial lines with a rigorous expansion method, it can

be shown that the two methods are equivalent through first order (the effect of curvature causing departure from constant property lines being of order $R^{-3/2}$). The great advantage of the current method is its simplicity in accounting for the dominant curvature effects and the fact that the flow field varies smoothly across the initial line (i.e., there are no sudden energy release changes or flow field adjustments downstream of the initial line caused by incompatibilities between the gas and chemical properties along the initial line). Thus inaccuracies in the initial line construction used in the present program do not cause physically unreal expansions, compressions or shocks in the characteristic calculations. This later advantage is extremely important since experience has shown that even small incompatibilities between the gas and chemical properties along the initial line can cause very large, physically unreal, flow field adjustments downstream of the initial line. The present method also conserves energy across the initial line which is only approximately conserved in other methods.

2.2.4 Constant Fraction Lag Relationships

The above method of constructing the particle properties makes use of the constant fractional lag relationships to relate the gas and particle flow fields. These relationships can be simply derived from the particle drag equations along particle streamlines.

$$u_{pi} \frac{du_{pi}}{dx} = \frac{9}{2} \frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2} (u - u_{pi}) \qquad (2\text{-}67)$$

$$u_{pi} \frac{dv_{pi}}{dx} = \frac{9}{2} \frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2} (v - v_{pi}) \qquad (2\text{-}68)$$

These equations can be rewritten as

$$K_i^2 \frac{du}{dx} + K_i u \frac{dK_i}{dx} = \frac{9}{2} \frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2} (1 - K_i) \qquad (2\text{-}69)$$

$$L_i \frac{dv}{dx} + \frac{dL_i}{dx} = \frac{9}{2} \frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2} \frac{1 - L_i}{K_i} \tan \theta \qquad (2\text{-}70)$$

where

$$K_i = \frac{u_{pi}}{u} \qquad (2\text{-}71)$$

$$L_i = \frac{v_{pi}}{v} \qquad (2\text{-}72)$$

In the throat region of a nozzle, the terms $\frac{u \, d K_i}{dx}$ and $\frac{v \, d L_i}{dx}$ are negligible compared to the other terms. Neglecting these terms the above equations can be solved for K_i and L_i where

$$K_i = \frac{9}{4} \frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2} \left(\frac{du}{dx}\right)^{-1} \left[\sqrt{1 + \frac{8}{9} \frac{m_{pi} r_{pi}^2}{\mu f_{pi} r^*} \frac{du}{dx}} - 1\right] \qquad (2\text{-}73)$$

$$L_i = \frac{9}{4} \frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2} \tan \theta_{pi} \left(\frac{dv}{dx}\right)^{-1} \left[\sqrt{1 + \frac{8}{9} \frac{m_{pi} r_{pi}^2}{\mu f_{pi} r^*} \cot \theta_{pi} \frac{dv}{dx}} - 1\right] \qquad (2\text{-}74)$$

Since

$$\tan \theta_{pi} = \frac{L_i}{K_i} \tan \theta \qquad (2\text{-}75)$$

one obtains by use of the above relationships

$$\frac{du}{dx} \left(\frac{dv}{dx}\right)^{-1} \left[\frac{\sqrt{1 + \frac{8}{9} \frac{m_{pi} r_{pi}^2}{\mu f_{pi} r^*} \cot \theta_{pi} \frac{dv}{dx}} - 1}{\sqrt{1 + \frac{8}{9} \frac{m_{pi} r_{pi}^2}{\mu f_{pi} r^*} \frac{du}{dx}} - 1}\right] \tan \theta = 1 \qquad (2\text{-}76)$$

which is Equation (2-58).

3. NUMERICAL INTEGRATION METHOD

The two-phase reacting gas characteristic relationships [Equations (2-18) through (2-31)] can be integrated using second order explicit methods which are generally simpler than implicit methods. It has been shown, however,[9] that implicit integration methods are superior to explicit methods for integrating chemical relaxation equations. The particle properties are also governed by equations of the relaxation type. Thus, in the present program, the fluid dynamic equations are integrated using an explicit modified Euler method while the particle and chemical relaxation equations are integrated using a first order implicit integration method.

In perfect gas flows, the flow is isentropic along streamlines and the streamline relasionships can be integrated in close form. Thus, in calculating supersonic perfect gas flow fields using the methods of characteristics, only the Mach line relationships need be numerically integrated to construct the flow field. In the calculation of supersonic reacting-gas flow fields, the flow is nonisentropic along streamlines and the streamline relationships must be numerically integrated as well as the Mach line relationships. In two-phase flows, the condensed phase does not follow the gas streamlines due to particle inertia and the calculation becomes even more complicated since a separate particle streamline must be considered for each particle present in the flow.

In numerical calculating flow fields using the method of characteristics only two (previously calculated) known points are directly usable in calculating a forward point. In nonequilibrium flows, however, more than two known points are required to calculate a forward point so that a choice must be made as to which points in the flow field will be used directly and which will be interpolated. In the reacting gas program,[10] the back streamline point and one characteristic point were chosen as the known points

since even small interpolation errors in species concentrations will cause serious stability and accuracy problems in the numerical integration of the chemical relaxation equations. This choice avoids interpolation for the species concentrations in that only the fluid dynamic properties (velocity, temperature, etc.) and the total entropy production term due to all nonequilibrium effects need to be interpolated at one of the back characteristic points. Since these quantities are all slowly varying across the characteristic mesh, they can be interpolated quite accurately. In the present two phase reacting gas nonequilibrium program, the same basic numerical methods are used by choosing as known points the gas streamline point and one characteristic point and interpolating for the other characteristic point and the particle streamline points. A complete derivation of the numerical methods used in the program are given in Sections 3.1, 3.2, and 3.3 below.

3.1 INTEGRATION OF THE FLUID DYNAMIC FQUATIONS

Consider the flow field shown in Figure 3-1.

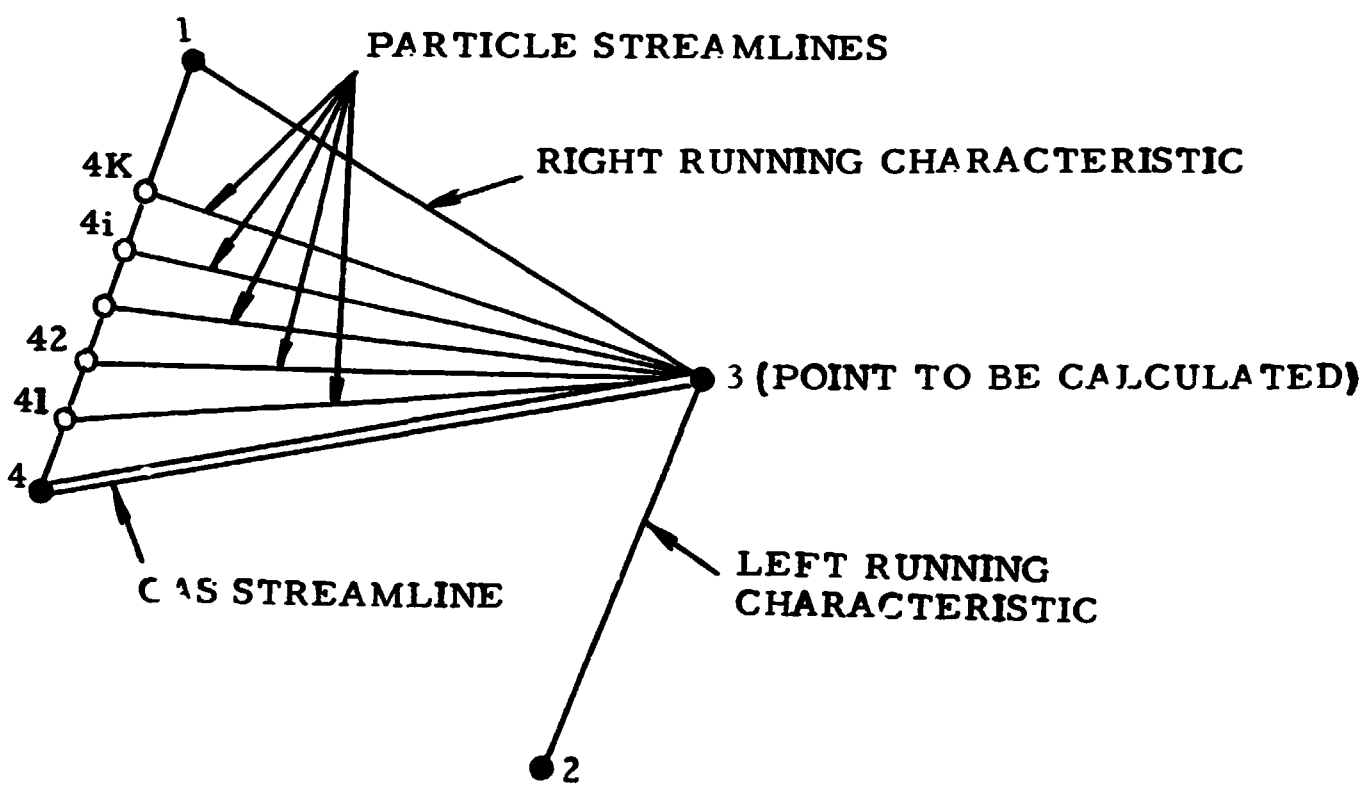

Figure 3-1. Flow Field Calculation

Between points 3 and 4, the gas streamline characteristic relationships are integrated as

$$r_3 = r_4 + \tan\left[\frac{1}{2}(\theta_4 + \theta_3)\right](x_3 - x_4) \qquad (3\text{-}1)$$

$$V_3 = \left\{V_4^2 + \frac{2N}{N-1}\frac{P_4}{\rho_4}\left[1 - \left(\frac{P_3}{P_4}\right)\frac{N-1}{N}\right] + \left(\frac{C_4}{\cos\theta_4} + \frac{C_3}{\cos\theta_3}\right)(x_3 - x_4)\right\}^{\frac{1}{2}} \qquad (3\text{-}2)$$

$$\rho_3 = \rho_4\left(\frac{P_4}{P_4}\right)^{\frac{1}{2}\left(\frac{1}{\gamma_4} + \frac{1}{\gamma_3}\right)} \exp\left[-\frac{1}{2}\left(\frac{A_4}{\cos\theta_4} + \frac{A_3}{\cos\theta_3}\right)(x_3 - x_4)\right] \qquad (3\text{-}3)$$

$$T_3 = T_4\left(\frac{P_3}{P_4}\right)^{\frac{1}{2}\left(\frac{\gamma_4 - 1}{\gamma_4} + \frac{\gamma_3 - 1}{\gamma_3}\right)} \exp\left[-\frac{1}{2}\left(\frac{B_4}{\cos\theta_4} + \frac{B_3}{\cos\theta_3}\right)(x_3 - x_4)\right] \qquad (3\text{-}4)$$

where

$$N = \frac{\ln\left(\frac{P_3}{P_4}\right)}{\ln\left(\frac{\rho_3}{\rho_4}\right)} \qquad (3\text{-}5)$$

The integration formula (3-1) relating the coordinates of points 3 and 4 was chosen since it is exact if the streamline is a circular arc between points 3 and 4. This is an excellent approximation over one mesh step. In integrating the momentum equation to obtain Equation (3-2), it was assumed that P varies as

ρ^N along the streamline. Equations (3-3) and (3-4) are obtained by using the energy equation and the equation of state. In obtaining formulas (3-2), (3-3), and (3-4), the coefficients [γ^{-1}, $(\gamma-1)/\gamma$, $A/\cos\theta$, $B/\cos\theta$, and $C/\cos\theta$] appearing in these equations were assumed to be equal to their average value between points 3 and 4. These integration formulas are exact for nonreacting, one-phase, constant-gamma flows (note that in this case N equals γ and A, B, and C are zero).

Between points 1 and 3 the right running characteristic relationships are integrated as

$$r_3 = r_1 + \tan\left[\frac{1}{2}(\theta_1 + \theta_3 - \alpha_1 - \alpha_3)\right](x_3 - x_1) \quad (3\text{-}6)$$

$$P_3 = P_1 \exp -\left[\frac{1}{2}(E_1G_1H_1 + E_3G_3H_3)(x_3 - x_1)\right.$$
$$- \frac{1}{2}\left(\frac{G_1H_1 \sin\theta_1}{r_1} + \frac{G_3H_3 \sin\theta_3}{r_3}\right)(x_3 - x_1)$$
$$\left. - \frac{1}{2}(G_1 + G_3)(\theta_3 - \theta_1)\right] \quad (3\text{-}7)$$

The integration formula (3-6) relating the coordinates of points 1 and 3 was chosen since it is exact if the right running characteristic is a circular arc between points 1 and 3. This is an excellent approximation over one mesh step. In integrating the right running characteristic relationship to obtain Equation (3-7) the coefficients (EGH, GH $\sin\theta/r$, and G) appearing in Equation (2-26) were assumed to equal their average value between points 1 and 3. This is an excellent approximation over one mesh step. If point 3 is an axis point then r_3 and $\sin\theta_3$ are zero and the indeterminate quantity $\sin\theta_3/r_3$ appearing in Equation (3-7) is approximated by

$$\frac{\sin \theta_3}{r_3} = \frac{\tan \theta_1}{r_1 + (x_3 - x_1) \tan \theta_1} \qquad (3\text{-}8)$$

Equation (3-8) is obtained by extrapolating for the ratio $\sin\theta/r$ on the axis, assuming that the flow near the axis is a source flow.

Between points 2 and 3, the left running characteristic relationships are integrated as

$$x_3 = x_2 + \cot\left[\frac{1}{2}(\theta_2 + \theta_3 + \alpha_2 + \alpha_3)\right](r_3 - r_2) \qquad (3\text{-}9)$$

$$P_3 = P_2 \exp\left[\frac{1}{2}(D_2G_2F_2 + D_3G_3F_3)(r_3 - r_2)\right.$$
$$- \frac{1}{2}\left(\frac{G_2F_2 \sin\theta_2}{r_2} + \frac{G_3F_3 \sin\theta_3}{r_3}\right)(r_3 - r_2)$$
$$\left. - \frac{1}{2}(G_2 + G_3)(\theta_3 - \theta_2)\right] \qquad (3\text{-}10)$$

The integration formula (3-9) relating the coordinates of points 2 and 3 was chosen because it is exact if the left running characteristic is a circular arc between points 2 and 3. This is an excellent approximation over one mesh step. In integrating the left running characteristic relationship to obtain Equation (3-10), the coefficients (DGF, GF $\sin\theta/r$, and G) appearing in Equation (2-24) were assumed to equal their average value between points 2 and 3. This is an excellent approximation over one mesh step. If point 2 is an axis point, then r_2 and θ_2 are zero and the indeterminate quantity $\sin\theta_2/r_2$ appearing in Equation (3-10) is that quantity previously calculated for the axis point using Equation (3-8).

Equations (3-7) and (3-10) can be combined to yield

$$\theta_3 = \frac{1}{G_3 + \frac{1}{2}(G_1 + G_2)} \left[\ln\left(\frac{P_2}{P_1}\right) + \frac{1}{2}(G_1 + G_3)\theta_1 + \frac{1}{2}(G_2 + G_3)\theta_2 \right.$$

$$+ \frac{1}{2}(D_2G_2F_2 + D_3G_3F_3)(r_3 - r_2)$$

$$- \frac{1}{2}\left(\frac{G_2F_2 \sin\theta_2}{r_2} + \frac{G_3F_3 \sin\theta_3}{r_3}\right)(r_3 - r_2)$$

$$+ \frac{1}{2}(E_1G_1H_1 + E_3G_3H_3)(x_3 - x_1)$$

$$\left. - \frac{1}{2}\left(\frac{G_1H_1 \sin\theta_1}{r_1} + \frac{G_3H_3 \sin\theta_3}{r_3}\right)(x_3 - x_1) \right] \quad (3\text{-}11)$$

In the various point calculations, Equation (3-11) is solved for θ_3 and either Equation (3-7) or (3-10) is solved for P_3, depending on whether point 1 or point 2 is the known data point.

It can be shown that use of these integration equations results in an error of order h^3 where h is the integration increment (mesh size). Since these integration equations involve the flow properties at the unknown point (point 3), they must be solved by iteration.

3.2 INTEGRATION OF THE CHEMICAL RELAXATION EQUATIONS

It has been shown by Tyson[1] that in the numerical integration of relaxation equations in near equilibrium flow regimes (such as the chamber and nozzle inlet in rocket engines), explicit integration methods are unstable unless the integration step size is of the order of the characteristic relaxation distance of the relaxation equations. Since the characteristic relaxation distance is orders of magnitude

smaller than the characteristic physical dimensions of the system of interest (such as the nozzle throat diameter and length) in near equilibrium flow regions, the use of explicit methods to integrate relaxation equations in these regions results in excessively long computation times. Implicit integration methods were shown to be inherently stable in integrating relaxation equations in all flow situations (whether near equilibrium or frozen) and can thus be used to integrate with step sizes of the order of the physical dimensions of the system of interest throughout the integration reducing the computation time per case several orders of magnitude. Since it has been demonstrated that there are significant advantages in using implicit rather than explicit integration methods for integrating relaxation equations, a first order implicit integration method has been chosen for use in the present program. A complete derivation of this numerical integration method is given below.

The chemical relaxation equations are a coupled set of first order simultaneous differential equations of the form

$$\frac{dc_i}{dx} = f_i(c_1, c_2, \cdots, c_N, y_1, y_2, y_3, y_4) \qquad i = 1, 2, \cdots, N \quad (3\text{-}12)$$

along the streamling where y_1, y_2, y_3, and y_4 refer to the fluid dynamic variables V, ρ, T, and θ, respectively. Assuming that the equations are not singular and that a solution exists which may be developed as a Taylor series about the forward point, one obtains

$$k_i = \left.\frac{dc_i}{dx}\right|_{x_n+h} h \qquad (3\text{-}13)$$

where k_i is the increment in c_i and h is sufficiently small. The first coefficient of the Taylor series may be calculated as

$$\frac{dc_i}{dx} = f_i(c_1, c_2, \cdots, c_N, y_1, y_2, y_3, y_4) \qquad (3\text{-}14)$$

Expanding them as a Taylor series about the point x_n, it is found that

$$\left.\frac{dc_i}{dx}\right|_{x_n+h} = f_{i,n} + \sum_{j=1}^{N} \beta_{i,j,n} k_j + \sum_{j=1}^{4} \phi_{i,j,n} \Delta y_j + 0\left[h^2\right] \quad (3\text{-}15)$$

where

$$\beta_{i,j} = \frac{\partial f_i}{\partial c_j} \quad (3\text{-}16)$$

$$\phi_{i,j} = \frac{\partial f_i}{\partial y_j} \quad (3\text{-}17)$$

and the subscript n refers to the functions f_i, $\beta_{i,j}$ and $\phi_{i,j}$ evaluated at the point x_n.

Substituting the above derivative into Equation (3-13) and neglecting the second order error and derivative terms yields the integration formula for the increment k_i.

$$k_i = \left[f_{i,n} + \sum_{j=1}^{N} \beta i,j,n \; k_j + \sum_{j=1}^{4} \phi_{i,j,n} \; \Delta y_j \right] h \quad (3\text{-}18)$$

3.3 INTEGRATION OF THE PARTICLE FLOW EQUATIONS

The equation relating the coordinates of an ith particle streamling [Equation (2-27)] can be integrated using second order explicit method. The integration formula is

$$r_3 = r_{4i} + \tan\left[\frac{1}{2}\left(\theta_{pi_{4i}} + \theta_{pi_{3i}}\right)\right](x_3 - x_{4i}) \quad (3\text{-}19)$$

which relates point 4i to point 3 (see Figure 3-1).

In calculating the particle density ρ_{pi} from Equation (2-19), it is convenient to use an integration formula obtained by making a mass balance between mesh points. By equating the mass flow

between points 4i and 2 to the mass flow between points 3 and 2 (there is no mass flow of ith particles between points 4i and 3 since these points are the ith particle streamline points), one obtains an integration formula for the density of the ith particle group at point 3.

$$\rho_{pi_3} = \left[u_{pi_3}(r_3^2 - r_2^2) - v_{pi_3}(x_3 - x_2)(r_3 + r_2)\right]^{-1}$$
$$\left\{\rho_{pi_{4i}}\left[u_{pi_{4i}}(r_{4i}^2 - r_2^2) - v_{pi_{4i}}(x_{4i}-x_2)(r_{4i}+r_2)\right]\right.$$
$$+ \rho_{pi_2}\left[u_{pi_2}(r_{4i}^2 - r_3^2) - v_{pi_2}(x_{4i} + x_2)(r_{4i} + r_2) + \right.$$
$$\left.\left. v_{pi_2}(x_3 - x_2)(r_3 + r_2)\right]\right\} \qquad (3\text{-}20)$$

For the particle velocities u_{pi} and v_{pi} and the particle enthalpies h_{pi}, the governing equations [Equations (2-28) to (2-30)] are of the relaxation type. Hence the implicit method employed in integrating for the chemical species is also used in integrating for u_{pi}, v_{pi}, and h_{pi}. Letting

$$\overline{f}_i = \frac{9}{2}\frac{\mu f_{pi} r^*}{m_{pi} r_{pi}^2 u_{pi}} \qquad (3\text{-}21)$$

$$\overline{g}_i = -\frac{3\mu g_{pi} r^*}{m_{pi} r_{pi}^2 u_{pi}}\frac{C_p}{c_{ppi} P_r} \qquad (3\text{-}22)$$

and using a formula parallel to Equation (3-13), one obtains

$$\Delta u_{pi} = \left[\overline{f}_i(u - u_{pi})\right]_{x_{pi}}^{x_{pi}+\Delta x_{pi}} \Delta x_{pi} \qquad (3\text{-}23)$$

$$\Delta v_{pi} = \left[\overline{f}_i(v - v_{pi})\right]_{x_{pi}}^{x_{pi}+\Delta x_{pi}} \Delta x_{pi} \qquad (3\text{-}24)$$

$$\Delta T_{pi} = \left[\bar{g}_i (T_{pi} - T)\right]_{x_{pi} + \Delta x_{pi}} \Delta x_{pi}, \quad T_{pi} \neq T_{pmi} \qquad (3\text{-}25)$$

$$\Delta h_{pi} = \left[C_{ppi} \bar{g}_i (T_{pmi} - T)\right]_{x_{pi} + \Delta x_{pi}} \Delta x_{pi}, \quad T_{pi} = T_{pmi} \qquad (3\text{-}26)$$

Equation (3-25) is used when the particle temperature is changing, and Equation (3-26) is used when the particle is in the state of solidification.

4. DISCUSSION

In developing a computer program based on the present analysis, three major parts are required: an one-dimensional two-phase reacting gas part, an axisymmetric two-phase transonic part and an axisymmetric two-phase characteristics part. The one-dimensional part, which is the One-Dimensional Two-Phase Reacting Gas Nonequilibrium Performance Program, is used to determine the properties in the nozzle throat region. These properties are used in constructing the transonic initial data line. This data line supplies the initial values in the characteristics calculations for the supersonic section of the nozzle. These three parts have been programmed for an IBM 7094 Mod II computer, but they have not been combined into a functioning program since the large size of the complete program necessitates an excessive number of overlays during program execution causing extremely long computer time per case (greater than one hour). With the advance of larger computers in the future, a practical working program can be developed using the present analysis.

REFERENCES

1. J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, Molecular Theory of Gases and Liquids, John Wiley and Sons, Inc., New York, 1954.

2. J. R. Kliegel, "Gas Particle Nozzle Flows," in Ninth International Symposium on Combustion, Academic Press, Inc., New York, 1963.

3. J. Courant and K. O. Friedricks, Supersonic Flow and Shock Waves, Interscience Publishers, Inc., New York, 1948.

4. P. I. Gold and C. T. Weekley, "Chemical Species and Chemical Reactions of Importance in Nonequilibrium Performance Calculations," 02874-6001-R000, TRW Systems, 6 December 1966.

5. J. R. Kliegel, V. Quan, S. S. Cherry, and H. M. Frey, "One-Dimensional Two-Phase Reacting Gas Nonequilibrium Performance Program," 02874-6005-R000, TRW Systems, 15 August 1967.

6. S. W. Benson and T. Fueno, "Mechanism of Atom Recombination by Consecutive Vibrational Deactivations," J. Chem. Physics 36, 1597 (1962).

7. J. R. Kliegel and V. Quan, "Convergent-Divergent Nozzle Flows," 02874-6002-R000, TRW Systems, 30 December 1966.

8. J. R. Kliegel and G. R. Nickerson, "Flow of Gas-Particle Mixtures in Axially-Symmetric Nozzles," in Detonation and Two-Phase Flow, edited by S. S. Penner and F. A. Williams, Academic Press, Inc., New York, 1962.

9. T. J. Tyson, "An Implicit Integration Method for Chemical Kinetics," 9840-6002-RU000, TRW Space Technology Laboratories, September 1964.

10. J. R. Kliegel, V. Quan, G. R. Nickerson, and J. E. Melde, "Axisymmetric Reacting Gas Nonequilibrium Performance Program," 02874-6004-R000, TRW Systems, 8 March 1967.