

NUMERICAL INVESTIGATIONS IN THE BACKFLOW  
REGION OF A VACUUM PLUME  
NAG8-201

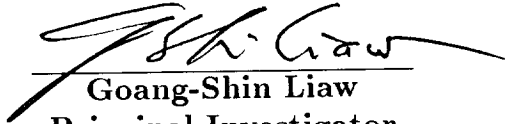
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# I. STATEMENT OF THE PROBLEM

## 1.1 Problem Definition and Method of Attack

The objective of this research work is to numerically simulate the vacuum plume flow field in the backflow region of a low thrust nozzle exit. In space applications, the low thrust nozzles are used as a propulsion device to control the vehicle attitude, or to maneuver the vehicle flight trajectory. When the spacecraft is deployed in the orbit or cruising in a planetary mission, the vacuum plume is created behind the nozzle exit (so called backflow region), by the exhausting gas of the propulsion system or by venting internal gas to the extremely low density ambient. The low density vacuum plume flow regions cover the continuum, transitional and free molecular flow regimes (see Figure 1), which were characterized by the Knudsen number  $K_n$ ,

$$K_n = \frac{\lambda_m}{L}$$

where  $\lambda_m$  is the mean free path of the gas molecules and  $L$  is the characteristic length of the flow field. Figure 1 shows the backflow regions determined by the  $K_n$  number. The transitional regime is defined by  $0.01 \leq K_n \leq 10$ . The conventional Navier-Stokes equations are valid only in the flow region close to the nozzle exit since the validity of the Navier-Stokes equations fails asymptotically as the Knudsen number increases. The vacuum plume characteristics prediction is primarily a problem of transitional aerodynamics.

In order to handle the rarefaction effects properly, the following hypothesis is made in this study,

“the Burnett equations are the governing equations in the transitional rarefied aerodynamic regime, where the Knudsen number is approximately between 0.01 and 10.”

This hypothesis is a compromise between the Boltzmann equation and the Navier-Stokes equations. Based on this hypothesis, the method to attack the vacuum plume problem in the backflow region is to develop a numerical technique to analyze the characteristics of the vacuum plume by solving the Burnett equations. For clarity, it is further assumed that the Navier-Stokes equations are no longer valid for this research problem, even though the Navier-Stokes equations are still approximately correct up to  $Kn = 10$  (Cheng, 1989). One of research objectives is to verify the consistency of the Burnett solutions with Navier-Stokes solutions and the Direct Simulation Monte Carlo solutions as well as the source flow correlation method in the transitional regime.

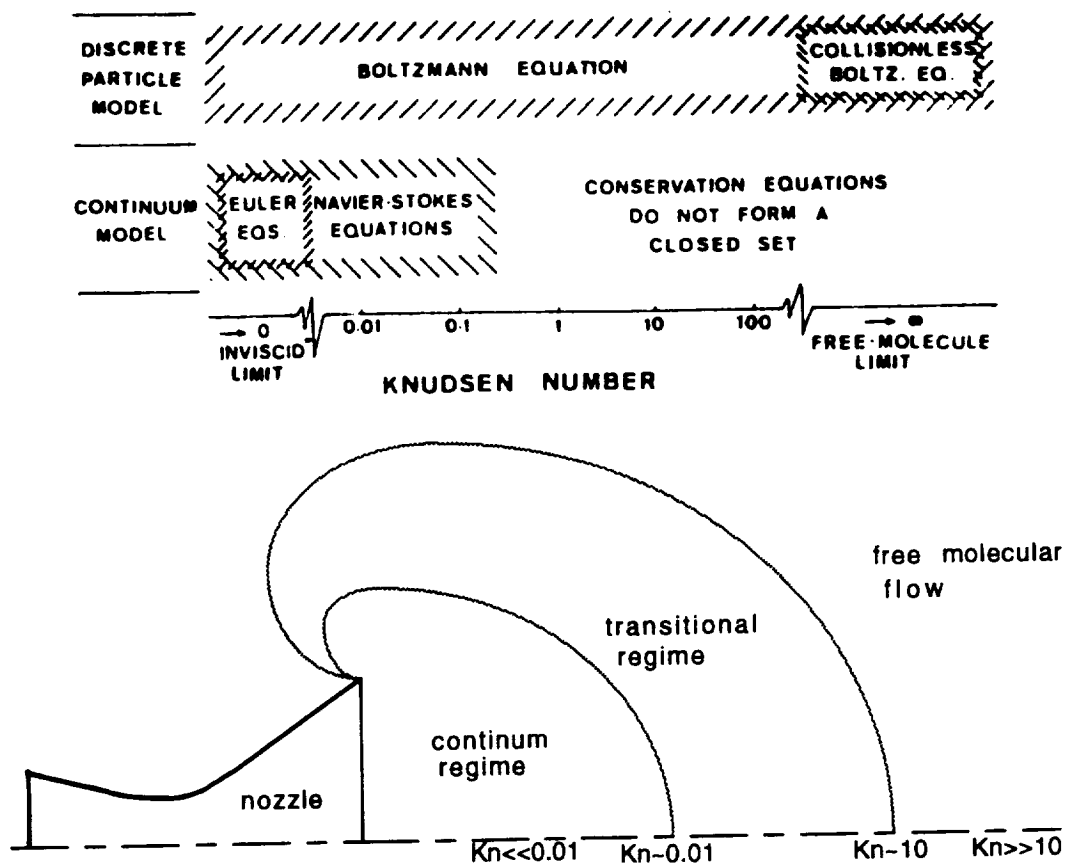


Figure 1. Schematic flow regimes in the backflow region and Validity of the Algorithms.

## 1.2 Survey of Low Density Nozzle/Space Plumes

Over the past years, many research efforts have been put into the space plume studies because the gasdynamics of this rarefied plume affects the vehicle trajectory control and propulsion efficiency. The plume in backflow region creates a negative force to the space vehicle, affects the vehicle torque control (Baerwald, 1978). Also the exhausted plume may contaminate the surface of the spacecraft. For the long duration flight, such as the Moon/Mars mission, an accurate definition of the vacuum plume is required for the improvement of the spacecraft performance.

It is difficult to simulate the space plume conditions by the ground test facility since it is very hard to pump the testing vacuum chamber pressure lower than 1 micron. It has been known that the performance of the low-thrust nozzle, unlike high thrust nozzle, is greatly affected by the back pressure in the testing vacuum chamber, even though the nozzle is operating under "choked" conditions. Available wind tunnel data show that, for a micropound thruster, if the back pressure falls into the region of 10 to 1000 microns, the thruster performance decreases with decreasing back pressure, however, the further decreasing of back pressure in the range of 0.1 to 10 microns will increase the thruster performance, (Pugmire 1968, John 1966, Sutherland 1966). There has been no proven theory in the exact cause of this "low pressure" anomaly. The numerical prediction is the only way to provide the answer.

The low density plume possesses the following characteristics (Kogan 1986, Legge 1988, Bird 1976): (1). The flow region covers the continuum, transitional, and free molecular flow regimes without solid boundaries; (2). The conventional Navier-Stokes equations are only valid close to the nozzle exit; (3). The translational nonequilibrium effects occur in the transitional regime; (4). There is no flow separation; (5). Transport properties not only depend on the first order spatial gradients of macroscopic flow variables, but also high order spatial gradients. These information indicate that the

vacuum (space) plume prediction is a problem of the transitional aerodynamics.

There have been many efforts towards solving backflow vacuum plume problems. The source flow technique developed by Boynton (1967) and Simons (1972) is a useful, inexpensive engineering design tool for the calculation of spacecraft impingement effects in the continuum regime, although some characteristics of the expansion are not properly treated. In order to produce a realistic source flow plume, the maximum Prandtl-Meyer expansion angle  $\theta_{max}$  is computed at the nozzle lip. Using this angle, the source flow area is computed as assuming the source to be located on the axis at a point defined by the interaction of the expansion angle with the axis. The model primarily assume that in the backflow plume region, the density at some radial distance from the source may be expressed as

$$\frac{\rho}{\rho_0} = \frac{A}{r^2} \cos^7 \left( \frac{\pi}{2} \frac{\theta}{\theta_{max}} \right) \quad .$$

where  $A$  is a plume constant, and, velocity may be assumed constant. The exponent 7 is obtained from the conservational mass and momentum. At the large distance from the nozzle exit, the flow may fall into transitional and free molecular regime, the gas is no longer in thermal equilibrium and the continuum equations become invalid. In order to understand detailed fluid dynamic phenomena in the backflow region, this empirical method can not produce successful results.

Method of Characteristics (MOC), plus the boundary layer prediction technique, can predict accurate plume expansion if Mach number is less than 10. For vacuum plume, the density is very low, the conventional MOC technique can still predict the flows, but the physical meaning and accuracy out of the computational number is in doubt.

Navier-Stokes equations have been widely accepted as a powerful and accurate governing equations for most continuum fluid flows. Most of the Navier-Stokes plume

predictions are performed at the low altitude where the density is fairly large compared to vacuum plume. Vacuum plume prediction is a problem of highly nonequilibrium transitional aerodynamic problem. In the discussion later, the Navier-Stokes equations fails in the transitional regime.

It is necessary to have new computational concepts (Direct Simulation of Monte Carlo technique) or governing equations (such as Burnett equations with nonequilibrium effects) in order to solve the complex transitional aerodynamics (vacuum plume in the backflow region), or a new numerical technique to solve the difficult physical equations (Boltzmann equation).



## II. TECHNICAL DISCUSSION

### 2.1 Introduction

From the physics point of view, the Boltzmann equation has long been established as the standard mathematical formulation of a nonequilibrium thermally perfect gas as a set of molecules. Whereas the continuum Navier-Stokes equations have the flow velocity and macroscopic thermodynamic properties as dependent variables. The only dependent variable in the Boltzmann equation is the distribution function for the molecular states. The velocity distribution function  $f$  is a scalar function which depends in general on time, the three components of molecular velocity, and the three components of molecular position,

$$f(u_i, x_i, t)du_i = \text{probability of molecule in velocity range } u_i + du_i, \\ \text{at position } x_i, \text{ at time } t$$

By taking moments (Lumpkin, 1990) of the velocity distribution function over all velocity space, all macroscopic thermodynamic properties of the gas can be obtained. However, the number of dependent variables is reduced at the expense of the additional number of independent variables from those of physical space to those of mathematical phase space. This leads to difficulties in the way of direct numerical or analytical solutions of Boltzmann equation for nontrivial gas flow problems though analytical solutions exist for a few simple cases. This applies even for monatomic gas flows and there is no prospect of obtaining direct solutions of the Boltzmann equation for complex aerothermodynamic problems involving real gas effects.

One alternative is to model the gas flow at the molecular level and a number of Monte Carlo simulation methods have been developed to do this. The Direct Simulation Monte Carlo (DSMC) method has gained a broad acceptance. Yet, while this method is capable of good predictions of hypersonic flow in the continuum transitional

regime, it is quite expensive in terms of computer time because the computational time is proportional to the molecules and cells number in the simulated flow. DSMC assumes that molecules are point centers of the mass and point centers of repulsion containing no internal structure. DSMC is primarily employed in highly rarefied gas flows, it is not practical to use DSMC for high Reynolds number flows in which Navier-Stokes equations can be solved instead. As a numerical technique, DSMC may be capable of predicting complex problems involving effects such as dissociation, chemical reactions, and radiation as long as the physics of the various phenomena can be described at the molecular level. However some essential physical questions concerning the continuum and transitional aerodynamic phenomena such as entropy are not answered satisfactorily.

To circumvent the vexed Boltzmann equation, an alternative can be achieved by solving conservational equations. To relate the nonequilibrium kinetic theory (Boltzmann equation) to the continuum theory of gas dynamics, Hilbert-Chapman-Enskog expansion method plays an important role. Based on this method, the velocity distribution function can be expressed in the series expansion of Knudsen number,

$$\begin{aligned}
 f &= f^{(0)} + f^{(1)} + f^{(2)} + f^{(3)} + \dots \\
 &= f^{(0)} (1 + a_1 K_n + a_2 K_n^2 + a_3 K_n^3 + \dots),
 \end{aligned}$$

which is the perturbation expansion of the velocity distribution function about the Maxwellian distribution which a gas exhibits at equilibrium, where  $f^{(0)}$  is the Maxwellian distribution function,  $a_i$ ,  $i = 1, 2, 3, \dots$  are functions of density, molecular velocity, and temperature (Bird, 1976). Substituting this expansion into Boltzmann equation, taking moments of the Boltzmann equation yields the continuum equations of fluid mechanics, a set of conservation equations describing global conservation of density, momentum, and energy. To close this system of equations requires constitutive equations which express viscous stress and heat flux in terms of the distribution function rather than macroscopic gradients. Closure of these equations can be achieved by using any of

the  $n$ th order approximations to the distribution function described in the expansion. The constitutive conditions relating viscous stress tensor and heat flux to macroscopic gradients can be obtained. By equating like terms for Knudsen number in Boltzmann equation, it was proved that the Euler equations are the zeroth-order approximation, the Navier-Stokes equations are the first-order approximation and the Burnett equations are the second-order approximation.

## 2.2 Inadequacy of the Navier-Stokes Equations

The conservation equations of fluid mechanics are valid in all flow regimes. But solving the general conservation equations (such as Navier-Stokes equations) require constitutive relations to close the system of equations. When the local Knudsen number which is based on the scale length of the gradients of the macroscopic flow properties exceeds 0.1, the conventional constitutive equations that relate the shear stress and heat fluxes to these gradients breakdown. One of the major breakdown in the transitional regime is that the thermal equilibrium fails.

Reasons for the failure of the Navier-Stokes equations may be associated with any or all of the following assumptions embodied in these equations (Fisko, 1989):

- (1). Linear stress-strain tensor dependent only on velocity gradients.
- (2). Linear heat-flux vector dependent only on temperature gradients.
- (3). Zero bulk viscosity.
- (4). Small Knudsen number flow (Continuum gas model).
- (5). No direct contribution of nonequilibrium internal molecular energy to viscous stress or heat flux.

## 2.3 Difficulties of Solving Burnett Equations

It has been a mislead concept that the Burnett equations are no more accurate than

the Navier-Stokes equations until Fisko and Chapman (1988) obtained the Burnett solutions for thick shocks. The comparison of solutions of Navier-Stokes, Burnett and the DSMC clearly shows that the Burnett solutions are superior to the Navier-Stokes solution (Figure 2). However, solving the Burnett equations is by no means a straightforward procedure because there are not enough well-defined boundary conditions for the fourth-order nonlinear partial differential equations. In addition, the questions of convergence, accuracy, stability, and viscous dissipation, etc., still remain.

Several fundamental questions are addressed in this report:

1. For tested monatomic gases and tested Mach numbers, the Burnett equations give a significant improvement over the Navier-Stokes equations in all macroscopic shock parameters as compared with DSMC and available experimental results (Lumpkin, 1990). But the flows in the transitional regime are always nonequilibrium. What is the theoretical ground to accept that the Burnett equations are the true governing equations in the transitional regime? The same question was raised towards the Boltzmann equation.
2. The mathematical characteristics of the Burnett equations are not clear, primarily because they are third-order highly nonlinear partial differential equations.
3. Most of the numerical schemes were developed for the Euler and Navier-Stokes equations. Should we routinely apply the numerical scheme to discretize the Burnett equations? What is the best stable numerical scheme to solve Burnett equations efficiently?
4. The boundary conditions for solving Burnett equations are undetermined.

As for this report, we are still working on the numerical scheme formulations and one-dimensional shock solutions in the wind tunnel conditions without answering these basic questions.

As a numerical experiment on Burnett equations, Direct Lower-Upper Factorization

(DLUF) scheme and the Arbitrary-Lagrangian-Eulerian (ALE) scheme have been developed and adopted to obtain the solutions for Burnett equations. The one-dimensional normal shock wave structures have been obtained by solving Navier-Stokes and Burnett equations, unsteady shock-tube solutions are also obtained from the ALE scheme. Difference between Navier-Stokes and Burnett solutions are shown for the density-temperature profiles for normal shock structure. The developed DLUF scheme shows a good potentials for solving Burnett equations will success. The ALE scheme has the advantages of reducing the order of partial differential equations, and allows more flexibility for viscous stress tensor and heat flux formulations.

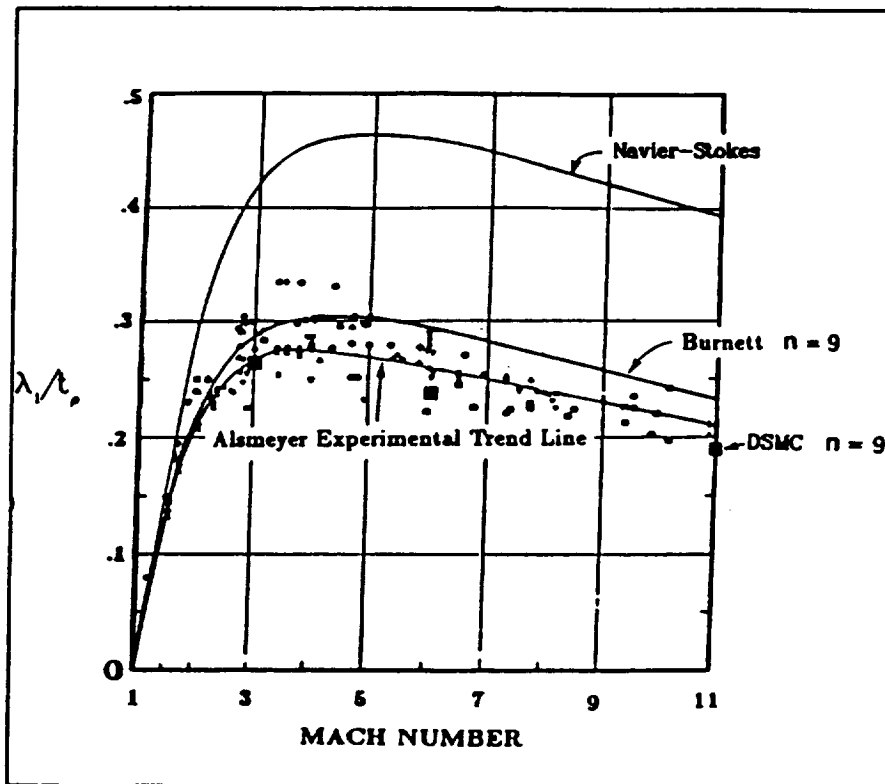


Figure 2. Comparison of reciprocal shock wave thickness by Navier-Stokes, Burnett, DSMC solutions and experiment.

## 2.4 Translational thermodynamic Nonequilibrium Effects

One of the major characteristic of vacuum plume flows is that the flow is always nonequilibrium, which primarily include the molecular translational, vibrational, and rotational nonequilibrium. For monatomic gases, the rotational and vibrational nonequilibrium are absent. Burnett equations do not account for molecular internal energy (i.e. rotation or vibration), and thus it is applied for monatomic gases. Since most of the gas is diatomic, attention must be given to the theory of the rotational and vibrational nonequilibrium effects. Unfortunately, the theory for rotational nonequilibrium is not as mature as the theory for translational nonequilibrium. This is due to the facts of complexity of the problem and lack of study interest.

In view of the theories up to date, it would seem that there are two basic ways to model rotational nonequilibrium effects using a continuum formulation. The first method, the so called “bulk viscosity” method, uses modifications to the stress tensor to account for the dissipation which results from rotational nonequilibrium. It assumes rapid equilibration and small departures from equilibrium, and is therefore inappropriate for hypersonic flow conditions. The second method, so called “relaxation equation” method, uses two temperatures to describe the rotational and translational energy modes. Since an additional temperature is used to describe the macroscopic state of the fluid, an additional governing equation is needed in addition to the conservation equations for mass, momentum, and energy. The additional governing equation can be derived from either the fully classical or the quasi-classical viewpoints. In both cases, the assumption of long relaxation times is required. The quasi-classical derivation also requires the assumption of small departure from equilibrium, an assumption which is not strictly valid in hypersonic flow. Comparing these two methods, for low density hypersonic flows, the relaxation equation method is preferred over a bulk viscosity method.

The general theory of translational-rotational nonequilibrium has only been carried out for first order departures from equilibrium distributions and in the limit of long relaxation times. The resulting set of equations (use both classical and quasi-classical models) is simply the Navier-Stokes equations supplemented by an additional governing equation, such as Jean's equation (Jean, 1904). The implementation of rotational nonequilibrium into Burnett equations, even for a monatomic gas, with the simplified modifications, is uncertain because of the accuracy of the additional governing equations is unknown for low density hypersonic flows.

the rotational and vibrational thermodynamic nonequilibrium excited in the high temperature, hypersonic flows are not important.

In this study, the interest is in the simulation of the backflow region, where low density effects is the major governing mechanism, the rotational and vibrational thermodynamic nonequilibrium excited in the high temperature hypersonic flows are not important. Therefore, our intention is to solve the monatomic gas problem such that translational nonequilibrium is the most important phenomena required to be accurately implemented. There are several attempts to analyze the translational nonequilibrium effects (Anderson, 1989). To handle the translational nonequilibrium, the translational and kinetic temperature have been introduced. Similarly, non-isotropic "pressure" (normal and tangential pressure) are used to evaluate the stress tensor. The key questions are still remaining: what is the relationship between these properties? What are the physical laws that guarantee the essential validity of these concepts? What are the appropriate boundary conditions?

## **2.5 Slip-Wall Conditions in Nozzle/Orifice Exit**

Due to the complexity of the physical problems, currently, the flows inside the low-thrust nozzle and vacuum plume are decoupled, in the sense that, the nozzle exit

conditions are used as the inflow boundary conditions for vacuum plume predictions. The specification of the nozzle exit conditions affects the accuracy of the vacuum plume predictions.

Theoretically, boundary conditions and, for unsteady flows, initial conditions must be given so as, in principle, to ensure the existence and uniqueness of the solution of the problem. However, in practical applications, the existence and uniqueness of the solution can not be proved and one must restore to physical intuition, non rigorous mathematical interpretation, and numerical experiments in order to determine the proper boundary conditions. The conventional wall boundary conditions, such as no-slip and no-temperature jump conditions, are only valid when  $K_n$  is less than 0.01. For low density nozzle, the nozzle expansion ratios are usually big enough that most likely, the flows at nozzle exit have very low densities such that  $K_n$  is greater than 0.01. In this case, the so-called “slip-wall” conditions need to be used at the nozzle wall exit. Based on kinetic theory, depending on the thermodynamic state and the laws of interactions between the gas molecules and the wall, the slip-wall conditions can be determined (Hollanders, 1988).

The flow variables along body (nozzle wall exit) surface ( $s$ ) can be computed by the first-order Maxwell/Smoluchowski (Kennard 1938, Schaaf 1961) slip boundary conditions (in Cartesian coordinates),

Surface velocity  $u_s$ ,

$$u_s = \frac{2 - R\sigma_n}{\sigma_n} \frac{2\mu}{\rho} \sqrt{\frac{\pi}{8RT}} \left( \frac{\partial u}{\partial y} \right)_s + \frac{3}{4} \frac{\mu}{\rho T} \left( \frac{\partial T}{\partial x} \right)_s,$$

and surface temperature  $T_s$ ,

$$T_s = T_w + \frac{2 - \sigma_t}{\sigma_t} \frac{2\gamma}{\gamma + 1} \frac{2\mu}{\rho P_r} \sqrt{\frac{\pi}{8RT}} \left( \frac{\partial T}{\partial y} \right)_s,$$

where  $T_w$  is the wall surface temperature,  $\sigma_n, \sigma_t$  are the surface reflection and accommodation factors, respectively. For a complete accommodation,  $\sigma_n = 1, \sigma_t = 1$ .



In order to treat rotational nonequilibrium effects, the above slip-wall boundary conditions can be extended as (Kennard 1938),

Surface velocity  $u_s$ ,

$$u_s = \frac{2 - R\sigma_n}{\sigma_n} \frac{2\mu}{\rho} \sqrt{\frac{\pi}{8RT}} \left( \frac{\partial u}{\partial y} \right)_s + \frac{3}{4} \frac{\mu}{\rho T} \left( \frac{\partial T}{\partial x} \right)_s$$

surface temperature  $T_s$ ,

$$T_s = T_w + \frac{2 - \sigma_t}{\sigma_t} \frac{3\lambda_t}{2\rho\bar{c}c_{vt}} \left( \frac{\partial T}{\partial y} \right)_s$$

and rotational surface temperature  $T_{rs}$ ,

$$T_{rs} = T_w + \frac{2 - \sigma_t}{\sigma_t} \frac{2\lambda_r}{\rho\bar{c}c_{vr}} \left( \frac{\partial T_r}{\partial y} \right)_s$$

where  $T_r$  is the rotational wall surface temperature,  $\lambda_t, \lambda_r$  are translational and rotational heat conductivity, respectively,  $C_{vt}, C_{vr}$  are translational and rotational specific heat per unit volume, and

$$\bar{c} = \sqrt{\frac{8RT}{\pi}}$$

### III. TECHNICAL ACHIEVEMENTS

#### 3.1 Reviews of the Burnett Equations

Literature survey on Burnett equations shows that only limited papers have been published on the derivation works. Chapman and Cowling (1970) derived the two-dimensional Burnett equations in Cartesian coordinates. Stanford's group, Chapman and Zhong et al. (1988, 1991), has systematically published their results in solving the Burnett equations.

In order to check the validity of the formulations, Burnett equations have been derived for one- and two-dimensional Cartesian coordinates. The final forms of the derivations (Liaw, Guo, 1992) is shown in Appendix.

#### 3.2 Pressure-Based Methodology (ALE Scheme)

In order to select a best numerical scheme to solve Burnett equations, extensive reviews on current existing TVD family of second-order central and upwind difference schemes have been performed. It is impossible to adopt a numerical scheme to solve Burnett equations without testing the capabilities of the specified scheme. Two different kinds of schemes have been examined/developed carefully, pressure-based methodology and density-based methodology.

The Arbitrary-Lagrangian-Eulerian (ALE) numerical technique is adopted in this investigation. The ALE scheme is a pressure-based methodology, which is a time-dependent finite volume differencing scheme for arbitrarily shaped geometry. In the current formulation, the gas could be chosen to be monatomic, diatomic or polyatomic arbitrarily. Due to the testing and validation purpose, the high order Burnett stress and heat flux terms are switched on only in one direction. For the present time, due to the limitation of time duration, the rotational and vibrational nonequilibrium for diatomic

of polyatomic gases are neglected.

The integrated mass, momentum, and energy equations over a moving control volume for gas/fluid may be written as

Continuity equation:

$$\frac{d}{dt} \iiint_{V(t)} \rho dV + \iint_{A(t)} \rho(\vec{u} - \vec{U}) \cdot d\vec{A} = 0$$

Momentum equations:

$$\frac{d}{dt} \iiint_{V(t)} \rho \vec{u} dV + \iint_{A(t)} \rho \vec{u}(\vec{u} - \vec{U}) \cdot d\vec{A} = - \iint_{A(t)} P d\vec{A} + \iint_{A(t)} \tau \cdot d\vec{A}$$

Energy equation:

$$\begin{aligned} \frac{d}{dt} \iiint_{V(t)} \rho E dV + \iint_{A(t)} \rho E(\vec{u} - \vec{U}) \cdot d\vec{A} &= - \iint_{c.s} P \vec{u} \cdot d\vec{A} \\ &+ \iiint_{V(t)} \tau : \nabla \vec{u} dV - \iint_{A(t)} \vec{J} \cdot d\vec{A} \end{aligned}$$

where

$$\begin{aligned} \vec{J} &= -k \nabla T - \rho D \sum_{m=1}^2 H_m \nabla \left( \frac{\rho_m}{\rho} \right) + J^{(2)} \\ \tau &= \mu (\nabla \vec{u} + (\nabla \vec{u})^T) + \lambda \nabla \cdot \vec{u} I + \tau^{(2)} \end{aligned}$$

where  $\rho$  is local fluid density,  $\vec{u}$  is local fluid velocity vector,  $\vec{U}$  is the moving boundary velocity,  $E$  is the specific internal energy not including chemical energy,  $P$  is static pressure,  $\tau$  is the viscous stress tensor,  $\tau^{(2)}$  is the Burnett stress tensor,  $\vec{J}$  is the heat flux vector,  $J^{(2)}$  is the Burnett heat flux vector,  $k$  is the thermal conductivity,  $\lambda$  and  $\mu$  are the dilatation and shear viscosity coefficients, respectively. The ideal gas equation of state is also assumed for the freestream gas.

At each cycle (time step), the calculations is divided into two stages, a Lagrangian stage and a rezone-Eulerian stage. In the Lagrangian stage, the velocities move with the fluid particle velocity, implicit differencing is used for all the diffusion terms and the terms associated with the pressure wave propagation. There is no convection across cell boundaries. The coupled implicit equations are solved by the method similar to the SIMPLE (Patankar, 1980) algorithm, with individual equations being solved by the conjugate gradient method (O'Rourke, 1986). In the rezone Eulerian stage, explicit methods are used to calculate convection. The convection calculation can be subcycled an arbitrary number of times, and thus the main computational timestep is not restricted by the Courant stability condition of explicit methods. A second-order upwind differencing technique is used for the spatial differencing. Detailed information about the ALE scheme can be found in Amsdan (1989) and Deng (1991).

The implementation of Burnett viscous stress and heat flux terms require special treatment of third-order partial differential terms and cross product terms of first-order second-order differentials. Due to the integration methodology, the order of partial differential terms in the formulations can be reduced by one. It is only necessary to define the viscous stress tensor and heat flux vector itself, which include only second-order partial differentials and cross product of first-order partial differentials. The basic methodology used here is based on the Gauss theorem, for any arbitrary scalar quantity  $Q$ ,

$$\iiint_V \frac{\partial Q}{\partial x_i} dV = \iint_A Q \hat{e}_i \cdot d\vec{A} = \sum_{\alpha=1}^4 Q_\alpha \hat{e}_i \cdot d\vec{A}_\alpha$$

By defining scalar property at the cell center, and vector property at cell vertex, it is possible to determine first-order partial derivatives at the cell surface, and second-order derivatives at the cell center.

### 3.2.1 Unsteady Shock-Tube Solutions by the ALE Scheme

To test the validity of the current scheme, a typical one-dimensional shock-tube solutions was obtained. The selected gas in this calculations was arbitrarily chosen to be Nitrogen. Rotational and vibrational nonequilibrium effects were neglected at the present time. The pressure ratio is 10 at the diaphragm initially. The shock tube length is 1m, the grid point along the tube is 201. The computed shock wave propagation at a given time from Euler, Navier-Stokes, and Burnett equations were compared to the exact Riemann solutions. The non-dimensional plots of pressure, density, velocity, and temperature are shown in Figure 3, 4 and 5. The computed results were based on real gas properties, which is currently defined in the way that all the thermodynamic properties such as viscosity, thermal conductivity, heat capacity, specific heat ratio, etc. are function of local temperature. Results shown at Figure 3 and 4 indicates that the current numerical scheme (ALE) predicts the shock wave propagation very accurately. The Burnett solutions is very close to the Navier-Stokes solutions in the way that only a small difference can be detected from data files. These results validate the current formulations.

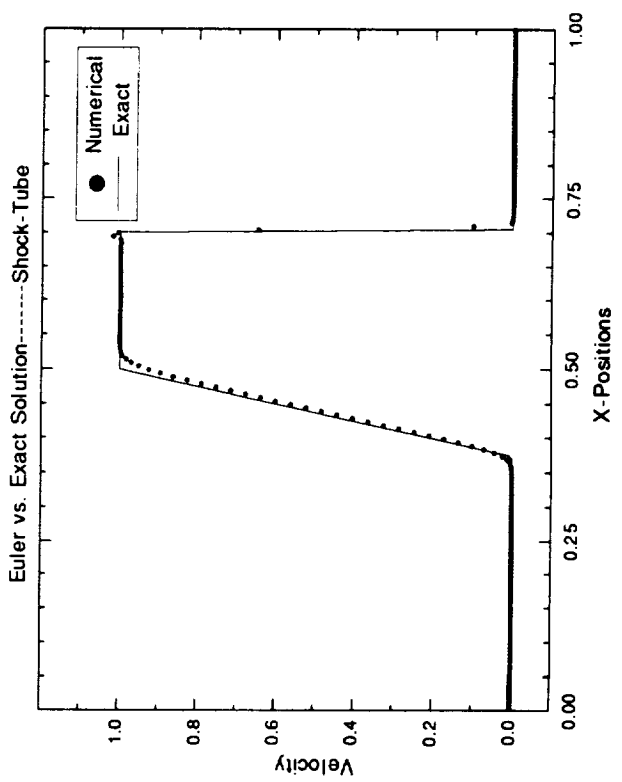
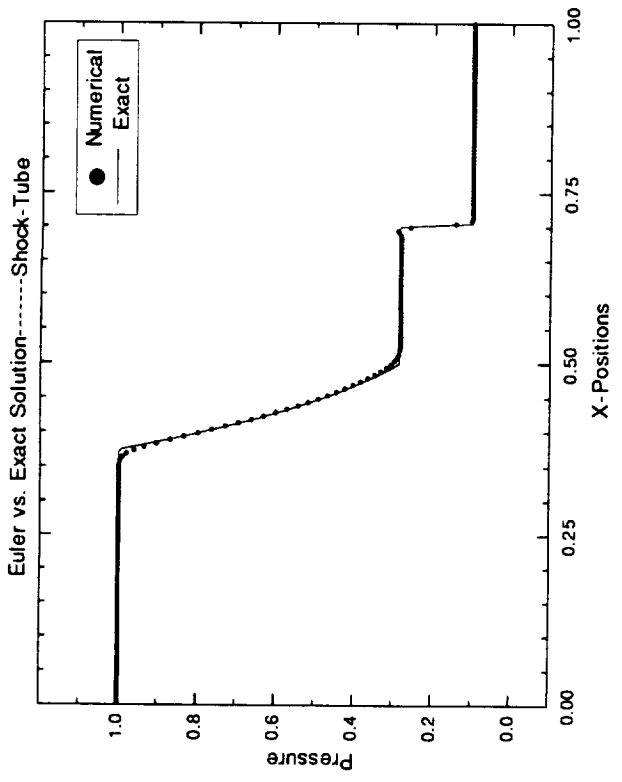
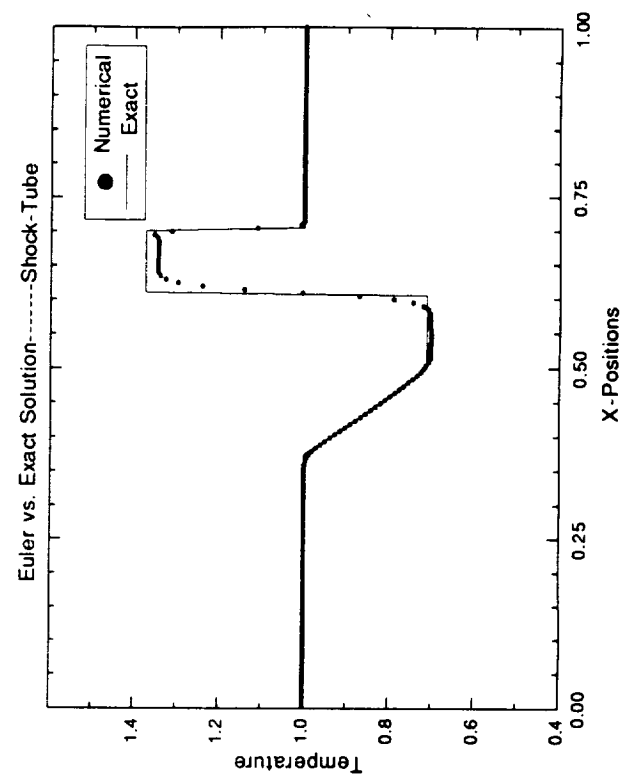
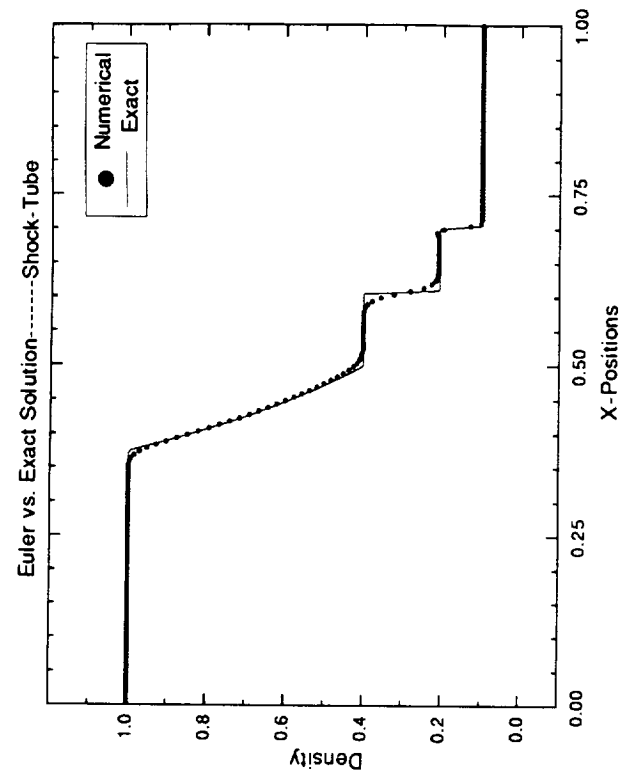


Figure 3. Comparison of Euler shock-tube solutions with exact solutions.

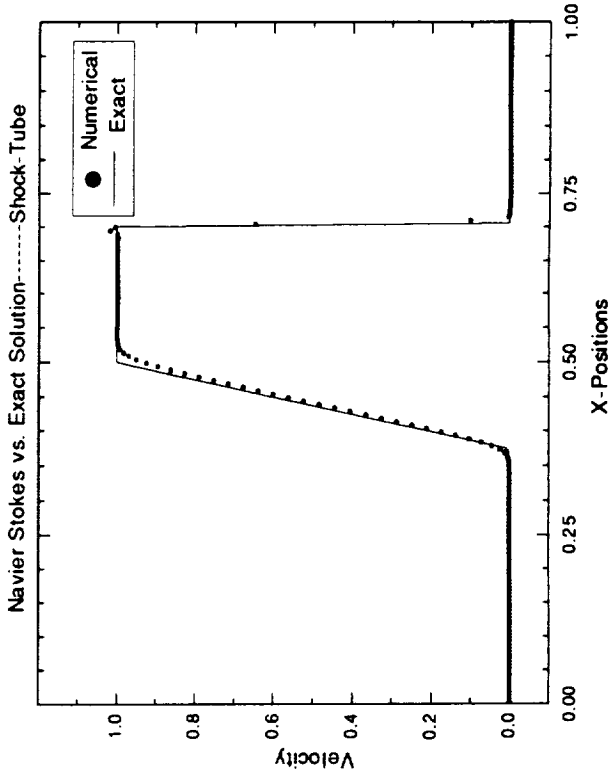
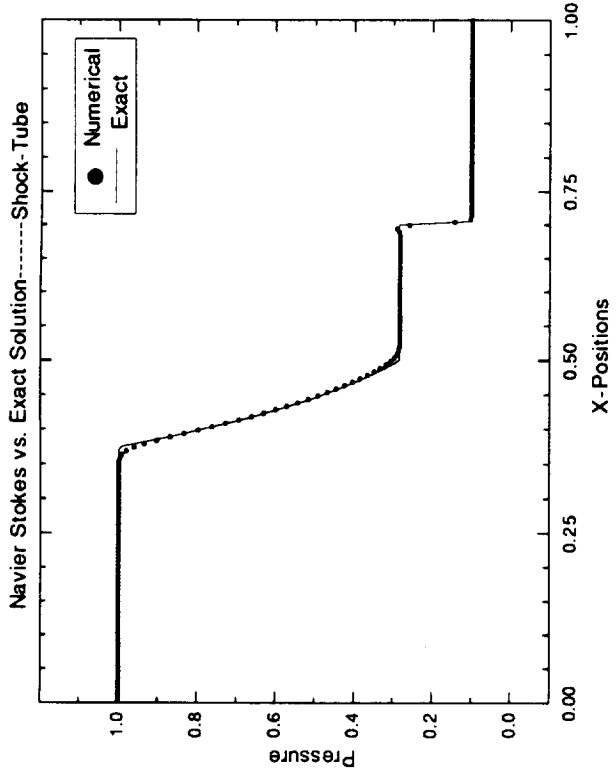
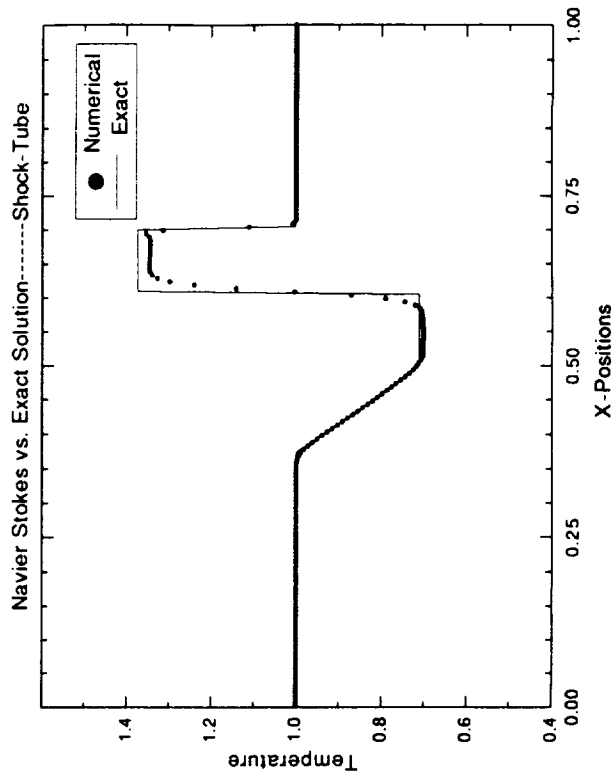
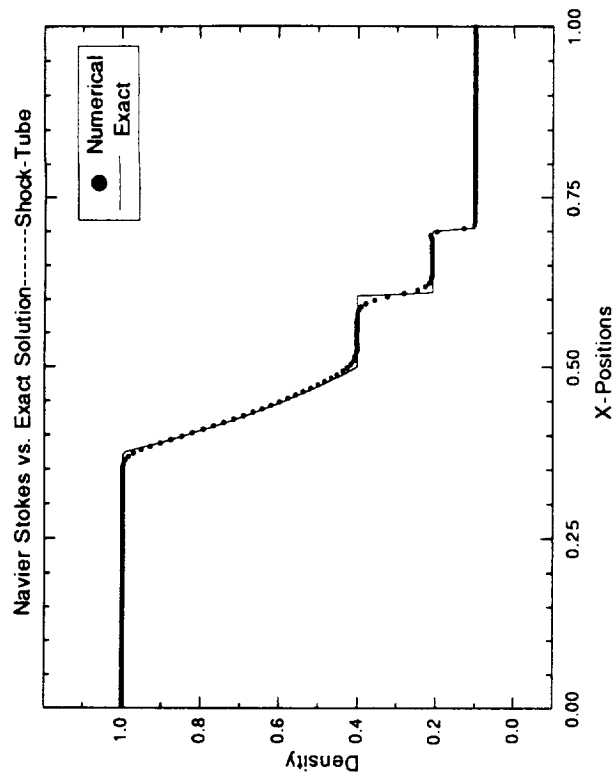


Figure 4. Comparison of Navier-Stokes shock-tube solutions with exact solutions.

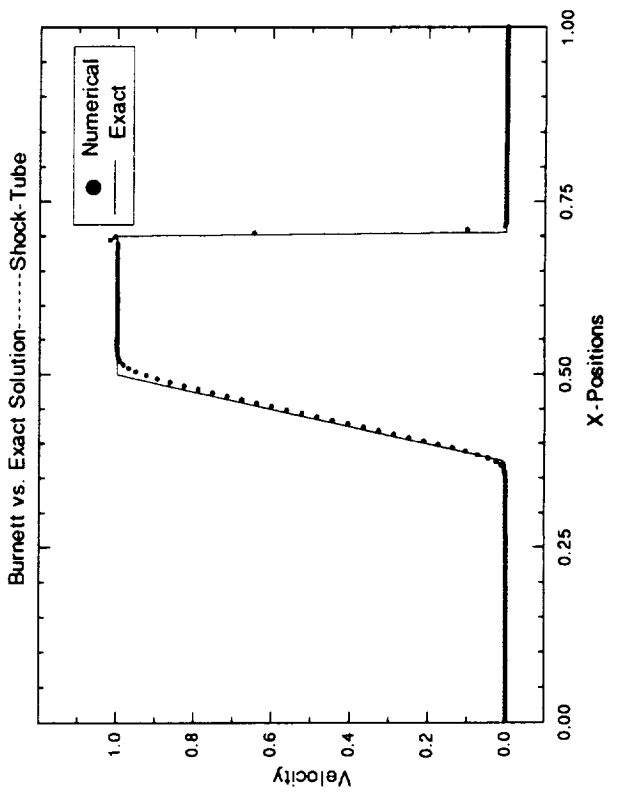
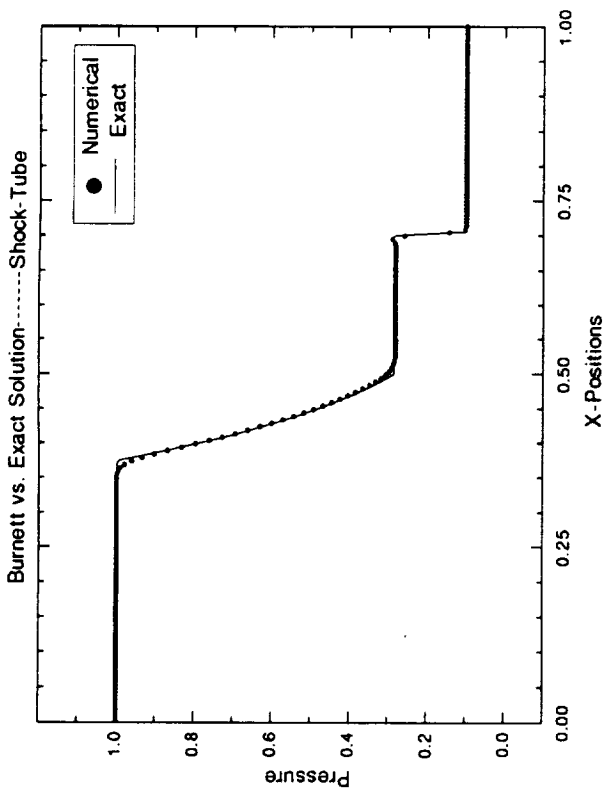
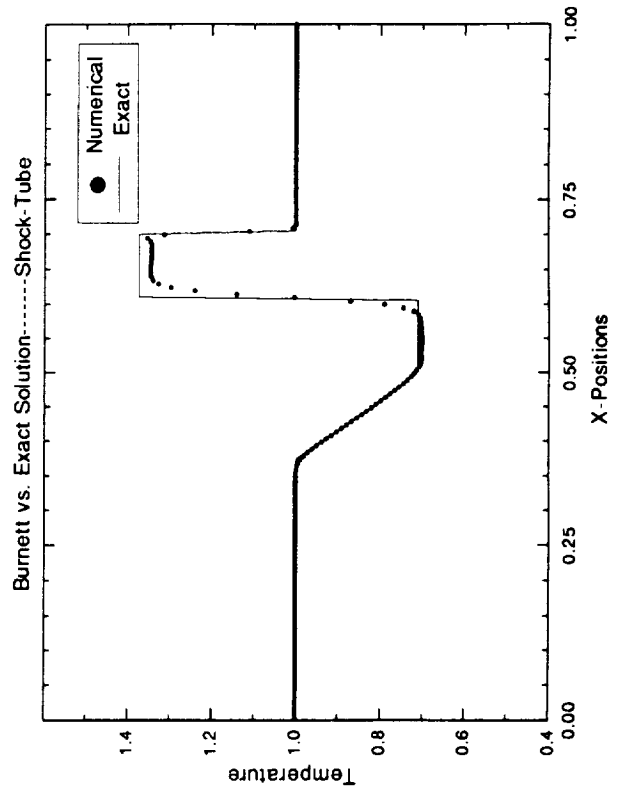
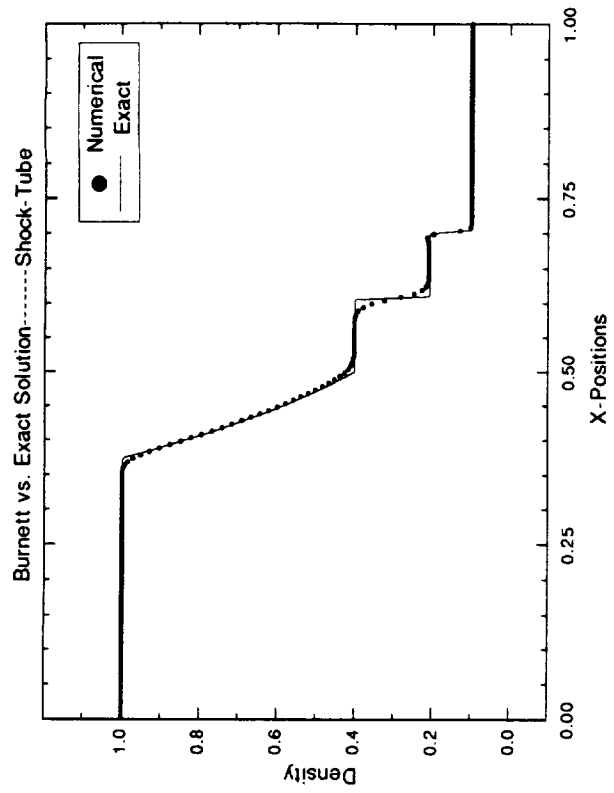


Figure 5. Comparison of Burnett shock-tube solutions with exact solutions.



### **3.2.2 Shock Wave Structures by the ALE Scheme**

High Mach number normal shock wave structure prediction is in progress. The comparison of Euler, Navier-Stokes, and Burnett solutions will be completed in the near future. The numerical experiments are for the Argon (monatomic) gas with different high inflow Mach numbers. Different scale calculations will be investigated.

## IV. FUTURE WORK

As mentioned in section one, the objective of this investigation is to find the flowfield in the vacuum plume backflow region in space. Three interrelated numerical techniques are proposed for the upcoming investigation.

1. The Burnett equations bridge the gaps between continuum and Boltzmann equation. The steady state solution of normal shock structure for Argon has been obtained by integrating the one-dimensional Burnett equations. The Direct Lower-Upper Factorization scheme is used to discretize the governing equations. More test conditions, primarily with lower densities and higher Mach numbers, will be exercised in this code. Preliminary results show that the Burnett terms suppress shock oscillations downstream, and it converges to the steady solution faster. The code development for two-dimensional flows will be continued in the future. The Direct Lower-Upper Factorization Scheme (DLUF) in two-dimensional rectilinear coordinates for Navier-Stokes/Burnett equations with a general grid generator will be developed. Under subcontract, Dr. J. D. Mo of the Memphis State University will be responsible for the basic code development. The principal investigator, Dr. G. S. Liaw of Alabama A&M University will be responsible for the insertion of the rarefaction effects and the nonequilibrium effects into the basic code. This new computer code will calculate the low density space-plume flowfield where the Knudsen number is less than 1. The ALE technique is also applied to solve Burnett equations. The numerical formulations are in the forms of three-dimensional fluid flows for real gases (monatomic, diatomic or polyatomic). Only one-dimensional cases has been validated. Continuous code development and validations for two- and three-dimensional cases will be performed in the future. The key questions here are how to handle the nonequilibrium effects. For monatomic gases, the rota-

tional and vibrational nonequilibrium are absent. Most of the real gases composed of the vacuum plume are diatomic or polyatomic. The future work towards solving Burnett equations including real gas effects will concentrate on the handling of the translational, rotational nonequilibrium effects.

2. For far field where the Knudsen number is larger than 1, the transitional nonequilibrium effects dominate the flow characteristics and continuum assumptions are in doubt. There are two approaches to tackle this problem:
  - (a). The Direct Simulation Monte Carlo (DSMC) technique,
  - (b). The Direct Solution of the Boltzmann Equation.

The DSMC is a straight forward and intuitive method to acquire the flowfield in large Knudsen number (Bird, 1990). The DSMC method is capable of simulating the low-density flow phenomena involving nonequilibrium of the translational and internal modes. Calculations can be made throughout the rarefied regimes and can overlap with the continuum calculations, the degree of overlap being dependent on the magnitude of the computing resources. It is very practical to adopt DSMC technique to attack the vacuum plume problems.

Direct solutions of Boltzmann equation have been a difficult subject for the aerodynamic problems (Cercignani, 1988). Based on literature survey, the only two-dimensional flow simulations based on direct solutions of Boltzmann equation was published by Tcheremissine (1989). However, direct solutions of Boltzmann equation in multidimensional flows require great computer resources as well as new numerical techniques. We plan to solve the nonlinear Boltzmann equation in the high Knudsen number backflow region of the plume using ALE technique. The appropriate upstream boundary conditions (close to the nozzle exit with relatively larger Knudsen number) will be provided by the solution of Burnett equations obtained by DLUF method. The solution of Boltzmann equation will provide indepth knowledge in classical sense of Hydrodynamics.

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## APPENDIX

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## Derivation of the Burnett Equations in Cartesian Coordinates

The Burnett equations in primitive variables are cast in the Cartesian tensor forms:

$$\frac{\partial \rho}{\partial t} + \rho_{,i} V_i + \rho V_{i,i} = 0 \quad (1)$$

$$\rho \frac{\partial V_i}{\partial t} + \rho V_j V_{i,j} + \sigma_{ij,j} = 0 \quad (2)$$

$$\rho \frac{\partial h}{\partial t} + \rho V_i h_{,i} - \frac{\partial p}{\partial t} - p_{,i} V_i - p V_{i,i} + \sigma_{ij} V_{j,i} + q_{i,i} = 0 \quad (3)$$

The constitutive relations for the viscous stress  $\sigma_{ij}$ , and heat flux  $q_{i,i}$ , are

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} + \cdots + \sigma_{ij}^{(k)} \quad (4)$$

$$q_i = q_i^{(0)} + q_i^{(1)} + q_i^{(2)} + \cdots + q_i^{(k)} \quad (5)$$

where  $i = 1, 2, 3$  and  $j = 1, 2, 3$ , and the superscript number  $k = 0, 1, 2, \dots, n$  represent the  $k$ th-order of accuracy.

- k=0,      the Euler equations,
- k=1,      the Navier-Stokes equations,
- k=2,      the Burnett equations,
- k=3,      the Super Burnett equations.

The viscous stress and heat flux, up to second-order terms, are described as follows:

$$\sigma_{ij}^{(0)} = p \delta_{ij} \quad (6)$$

$$\sigma_{ij}^{(1)} = -2\mu (D_{ij} - \frac{1}{3} D_{\alpha\alpha} \delta_{ij}) \quad (7)$$

$$\begin{aligned} \sigma_{ij}^{(2)} = & \frac{\mu^2}{p} \left\{ \omega_1 \frac{\partial u_\alpha}{\partial x_\alpha} (D_{ij} - \frac{1}{3} D_{\alpha\alpha} \delta_{ij}) + \omega_2 (L_{ij} - \frac{1}{3} L_{\alpha\alpha} \delta_{ij}) \right. \\ & \left. - \omega_2 (M_{ij} - \frac{1}{3} M_{\alpha\alpha} \delta_{ij}) - 2\omega_2 (N_{ij} - \frac{1}{3} N_{\alpha\alpha} \delta_{ij}) \right\} \end{aligned}$$

$$\begin{aligned}
& + \omega_3 R(A_{ij} - \frac{1}{3}A_{\alpha\alpha}\delta_{ij}) + \omega_4 \frac{1}{\rho T}(B_{ij} - \frac{1}{3}B_{\alpha\alpha}\delta_{ij}) \\
& + \omega_5 \frac{R}{T}(C_{ij} - \frac{1}{3}C_{\alpha\alpha}\delta_{ij}) + \omega_6(E_{ij} - \frac{1}{3}E_{\alpha\alpha}\delta_{ij}) \} \tag{8}
\end{aligned}$$

$$q_i^{(0)} = 0 \tag{9}$$

$$q_i^{(1)} = -\lambda \frac{\partial T}{\partial x_i} \tag{10}$$

$$\begin{aligned}
q_i^{(2)} = & \frac{\mu^2}{\rho} \{ \theta_1 \frac{1}{T} \frac{\partial T}{\partial x_i} \frac{\partial u_\alpha}{\partial x_\alpha} + \theta_2 \frac{1}{T} [ \frac{2}{3} \frac{\partial}{\partial x_i} (T \frac{\partial u_\alpha}{\partial x_\alpha}) + 2 \frac{\partial T}{\partial x_\alpha} \frac{\partial u_\alpha}{\partial x_i} ] \\
& + \theta_3 \frac{1}{p} \frac{\partial p}{\partial x_\alpha} (D_{\alpha i} - \frac{1}{3}D_{\lambda\lambda}\delta_{\alpha i}) + \theta_4 \frac{\partial}{\partial x_\alpha} (D_{\alpha i} - \frac{1}{3}D_{\lambda\lambda}\delta_{\alpha i}) \\
& + \theta_5 \frac{1}{T} \frac{\partial T}{\partial x_\alpha} (D_{\alpha i} - \frac{1}{3}D_{\lambda\lambda}\delta_{\alpha i}) \}, \tag{11}
\end{aligned}$$

where

$$D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{12}$$

$$L_{ij} = \frac{1}{2} \frac{\partial}{\partial x_i} \left( -\frac{1}{\rho} \frac{\partial p}{\partial x_j} \right) + \frac{1}{2} \frac{\partial}{\partial x_j} \left( -\frac{1}{\rho} \frac{\partial p}{\partial x_i} \right) \tag{13}$$

$$M_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_\alpha} \frac{\partial u_\alpha}{\partial x_j} + \frac{\partial u_j}{\partial x_\alpha} \frac{\partial u_\alpha}{\partial x_i} \right) \tag{14}$$

$$N_{ij} = \frac{1}{2} \left[ \frac{\partial u_\alpha}{\partial x_i} (D_{\alpha j} - \frac{1}{3}D_{\lambda\lambda}\delta_{\alpha j}) + \frac{\partial u_\alpha}{\partial x_j} (D_{\alpha i} - \frac{1}{3}D_{\mu\mu}\delta_{\alpha i}) \right] \tag{15}$$

$$A_{ij} = \frac{\partial^2 T}{\partial x_i \partial x_j} \tag{16}$$

$$B_{ij} = \frac{1}{2} \left( \frac{\partial p}{\partial x_i} \frac{\partial T}{\partial x_j} + \frac{\partial p}{\partial x_j} \frac{\partial T}{\partial x_i} \right) \tag{17}$$

$$C_{ij} = \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_j} \tag{18}$$

$$E_{ij} = (D_{i\alpha} - \frac{1}{3}D_{\lambda\lambda}\delta_{i\alpha})(D_{j\alpha} - \frac{1}{3}D_{\mu\mu}\delta_{j\alpha}). \tag{19}$$

where  $\omega_i$  and  $\theta_i$  can be determined by Chapman-Enskog method, depending on the gas molecular repulsive force models used. Expand the tensor terms from above equations in terms of the primitive variables and its derivatives, an explicit expression for the stress tensor components and heat flux vector components can be obtained.