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THEORETICAL STUDIES OF A MOLECULAR BEAM GENERATOR

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NOZZLE FLOW WITH VIBRATIONAL NONEQUILIBRIUM

Introduction

We consider the problem of modeling a high temperature diatomic gas N_2 flowing through a converging-diverging high expansion nozzle. The problem is modeled in two ways. The first model uses a single temperature with variable specific heats as functions of this temperature. For the second model we assume that the various degrees of freedom all have a Boltzmann population distribution which means that each degree of freedom has its own temperature and consequently each system state can be characterized by these temperatures. This suggests the formulation of a second model with a vibrational degree of freedom as having its own temperature along with a rotational-translational degree of freedom with its own temperature. Initially the vibrational degree of freedom is excited by heating the gas to a high temperature. As the high temperature gas expands through the nozzle throat there is a sudden drop in the rotational-translational temperature along with a finite relaxation time for the vibrational degree of freedom to achieve equilibrium with the rotational-translational degree of freedom. That is, the temperature change that occurs when the N_2 gas passes through the nozzle throat is so great that the changes in the vibrational degree of freedom lags behind the rotational-translational energy changes. The resulting relaxation time is finite. It is in this context that the term nonequilibrium is used. That is, the term nonequilibrium denotes the fact that the energy content of the various degrees of freedom are characterized by two temperatures. We neglect any chemical reactions resulting from the high temperatures which could also add nonequilibrium effects.

We develop the basic equations for the two models in various forms in order to check the derivations with other sources, references [1],[2]. The final form which is solved numerically are the scaled equations in a conservative dimensionless form.

Single Temperature Model

For our first model we assume that there exits a single temperature T which characterizes the energy state of the system. Using the list of symbols given in the Appendix A, the basic equations describing the flow through a nozzle with cylindrical symmetry are given by

$$\text{Continuity} \qquad \frac{D\varrho}{Dt} + \varrho\nabla\cdot\vec{V} = 0 \tag{1}$$

$$\text{Momentum} \qquad \varrho\frac{D\vec{V}}{Dt} = +\nabla\cdot(\mathbf{P}) \tag{2}$$

$$P_{ij} = -P\delta_{ij} + \eta(V_{i,j} + V_{j,i}) + \lambda\delta_{ij}(\nabla\cdot\vec{V}) \tag{3}$$

$$\text{Energy} \qquad \varrho\frac{\partial e}{\partial t} + \varrho\vec{V}\cdot\nabla e + P\nabla\cdot\vec{V} + \nabla\cdot\vec{q} = \frac{\partial Q}{\partial t} + \Phi \tag{4}$$

$$\text{Equation of State} \qquad P = \varrho RT \tag{5}$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{V} \cdot \nabla$ is the material derivative and

$$\vec{q} = q_r \widehat{\mathbf{e}}_r + q_z \widehat{\mathbf{e}}_z, \qquad \vec{V} = V_r \widehat{\mathbf{e}}_r + V_z \widehat{\mathbf{e}}_z \tag{6}$$

$$q_r = -K\frac{\partial T}{\partial r}, \qquad q_z = -K\frac{\partial T}{\partial z} \tag{7}$$

$$C_v = C_{vrt} + C_{vv}, \quad C_{vrt} = 5R/2, \quad C_{vv} = R\left(\frac{\phi}{T}\right)^2 \frac{e^{\phi/T}}{(e^{\phi/T}-1)^2}, \quad \phi = h\nu/k \tag{8}$$

$$e(T) = \int_{T_0}^{T} C_v\, dT = \frac{5}{2}R(T - T_0) + \frac{R\phi}{e^{\phi/T}-1} - \frac{R\phi}{e^{\phi/T_0}-1} \tag{9}$$

We assume that the external heat sources Q are zero. The symbol ϕ denotes the characteristic vibrational temperature which is unique for each gas species. For N_2 we use $\phi = 3395\,^\circ K$. For small temperatures we have $C_v \approx 5R/2$ so that the vibrational degree of freedom only becomes excited when the temperature is on the order of magnitude of ϕ. The coefficients of viscosity η and $\lambda = -2\eta/3$ are determined from the Sutherland formula, reference [3] where

$$\eta = \frac{c_1 g_c T^{3/2}}{T + c_2} \tag{10}$$

where for N_2 we use $c_1 = 1.488 * 2.16(10^{-8})$, $g_c = 32.174$, and $c_2 = 184.0$. The units of viscosity are $kg/m - sec$ when the temperature T is given in Rankine units. The quantity Φ represents the dissipation function and is given by

$$\Phi = \nabla(\tau_{ij}V_j) - \vec{V} \cdot \nabla(\tau_{ij}) = (\tau_{ij}V_j)_{,i} - V_i \tau_{ij,j} \tag{11}$$

where τ_{ij} are the viscous stress terms given by

$$\tau_{ij} = \eta(V_{i,j} + V_{j,i}) + \lambda \delta_{ij} \nabla \cdot \vec{V}. \tag{12}$$

The coefficient of thermal conductivity K is written, reference [4]

$$K = K_{rt} + K_v = \frac{\eta C_{p,rt}}{P_r} + \frac{\eta C_{vv}}{S_c} \tag{13}$$

where P_r is the Prandtl number and S_c is the Schmidt number. For N_2 at $0\,^\circ K$, we have the approximations $P_r \approx 0.71$ and $S_c \approx 0.74$. These values remain constant over a wide range of temperatures and produce the approximations

$$K_{rt} \approx 4.93\eta R \qquad K_v \approx 1.35\eta C_{vv}. \tag{14}$$

Computational Coordinates

The basic equations (1) through (5) are written in the weak conservative form,
Continuity

$$\frac{\partial \varrho}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\varrho V_r) + \frac{\partial(\varrho V_z)}{\partial z} = 0 \tag{15}$$

Momentum

$$\frac{\partial}{\partial t}(\varrho V_r) + \frac{1}{r}\frac{\partial}{\partial r}(r[\varrho V_r^2 + P - \tau_{rr}]) + \frac{\partial}{\partial z}(\varrho V_r V_z - \tau_{rz}) - \frac{P}{r} + \frac{\tau_{\theta\theta}}{r} = 0 \tag{16}$$

$$\frac{\partial}{\partial t}(\varrho V_z) + \frac{1}{r}\frac{\partial}{\partial r}(r[\varrho V_r V_z - \tau_{rz}]) + \frac{\partial}{\partial z}(\varrho V_z^2 + P - \tau_{zz}) = 0 \tag{17}$$

Energy

$$\frac{\partial E_t}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r[(E_t+P)V_r - V_r\tau_{rr} - V_z\tau_{rz} + q_r]) + \frac{\partial}{\partial z}((E_t+P)V_z - V_r\tau_{rz} - V_z\tau_{zz} + q_z) = 0 \tag{18}$$

Equation of State

$$P = \varrho RT \tag{19}$$

where E_t is the total energy per unit volume

$$E_t = \varrho e + \frac{\varrho}{2}(V_r^2 + V_z^2) \tag{20}$$

and the stresses given by

$$\tau_{rr} = 2\eta\frac{\partial V_r}{\partial r} + \lambda\nabla\cdot\vec{V} \tag{21}$$

$$\tau_{zz} = 2\eta\frac{\partial V_z}{\partial z} + \lambda\nabla\cdot\vec{V} \tag{22}$$

$$\tau_{\theta\theta} = 2\eta\frac{V_r}{r} + \lambda\nabla\cdot\vec{V} \tag{23}$$

$$\tau_{rz} = \tau_{zr} = \eta\left(\frac{\partial V_z}{\partial r} + \frac{\partial V_r}{\partial z}\right) \tag{24}$$

$$\nabla\cdot\vec{V} = \frac{1}{r}\frac{\partial}{\partial r}(rV_r) + \frac{\partial V_z}{\partial z} \tag{25}$$

and e is the internal energy per unit mass determined from the relation

$$de = C_v\, dT. \tag{26}$$

The internal energy per unit mass e is given by equation (9).

The equations (15) through (19) are to be solved over the solution domain $0 \leq z \leq b$, $0 \leq r \leq f(z)$ where $f(z)$ defines the shape of the nozzle. We introduce the dimensionless variables

$$r^* = \frac{r}{\delta} \quad z^* = \frac{z}{L} \quad t^* = \frac{t}{L/V_0} \quad V_r^* = \frac{V_r}{V_0\delta/L} \quad V_z^* = \frac{V_z}{V_0}$$
$$\varrho^* = \frac{\varrho}{\varrho_0} \quad \eta^* = \frac{\eta}{\eta_0} \quad P^* = \frac{P}{\varrho_0 V_0^2} \quad T^* = \frac{T}{T_0} \quad e^* = \frac{e}{V_0^2} \tag{27}$$

where L,δ are characteristic lengths, V_0 a characteristic velocity, ρ_0 a characteristic density, η_0 a characteristic viscosity, and T_0 is a characteristic temperature. There then results the dimensionless equations

Continuity

$$\frac{\partial \varrho^*}{\partial t^*} + \frac{1}{r^*}\frac{\partial}{\partial r^*}(r^*\varrho^* V_r^*) + \frac{\partial(\varrho^* V_z^*)}{\partial z^*} = 0 \tag{28}$$

Momentum

$$\frac{\partial}{\partial t^*}(\varrho^* V_r^*) + \frac{1}{r^*}\frac{\partial}{\partial r^*}(r^*[\varrho^* V_r^* V_r^* + \frac{L^2}{\delta^2}P^* - \frac{L^2}{\delta^2}\tau_{rr}^*/Re])$$
$$+ \frac{\partial}{\partial z^*}(\varrho^* V_r^* V_z^* - \frac{L^2}{\delta^2}\tau_{rz}^*/Re) - \frac{L^2}{\delta^2}\frac{P^*}{r^*} + \frac{L^2}{\delta^2}\frac{\tau_{\theta\theta}^*}{r^* Re} = 0 \tag{29}$$

$$\frac{\partial}{\partial t^*}(\varrho^* V_z^*) + \frac{1}{r^*}\frac{\partial}{\partial r^*}(r^*[\varrho^* V_r^* V_z^* - \frac{L^2}{\delta^2}\tau_{rz}^*/Re])$$
$$+ \frac{\partial}{\partial z^*}(\varrho^* V_z^* V_z^* + P^* - \tau_{zz}^*/Re) = 0 \tag{30}$$

Energy

$$\frac{\partial E_t^*}{\partial t^*} + \frac{1}{r^*}\frac{\partial}{\partial r^*}(r^*[(E_t^* + P^*)V_r^* - V_r^*\tau_{rr}^*/Re - \frac{L^2}{\delta^2}V_z^*\tau_{rz}^*/Re + q_r^*])$$
$$+ \frac{\partial}{\partial z^*}((E_t^* + P^*)V_z^* - V_r^*\tau_{rz}^*/Re - V_z^*\tau_{zz}^*/Re + q_z^*) = 0 \tag{31}$$

Equation of State

$$P^* = \varrho^* R T^*(T_0/V_0^2) \tag{32}$$

where E_t^* is the scaled total energy per unit volume

$$E_t^* = \varrho^* e^* + \frac{\varrho^*}{2}(\frac{\delta^2}{L^2}(V_r^*)^2 + (V_z^*)^2) \tag{33}$$

and the stresses given by

$$\tau^*_{rr} = 2\eta^* \frac{\partial V^*_r}{\partial r^*} + \lambda^* \nabla^* \cdot \vec{V^*} \tag{34}$$

$$\tau^*_{zz} = 2\eta^* \frac{\partial V^*_z}{\partial z^*} + \lambda^* \nabla^* \cdot \vec{V^*} \tag{35}$$

$$\tau^*_{\theta\theta} = 2\eta^* \frac{V^*_r}{r^*} + \lambda^* \nabla^* \cdot \vec{V^*} \tag{36}$$

$$\tau^*_{rz} = \tau^*_{zr} = \eta^* \left(\frac{\partial V^*_z}{\partial r^*} + \frac{\delta^2}{L^2} \frac{\partial V^*_r}{\partial z^*} \right) \tag{37}$$

$$\nabla^* \cdot \vec{V^*} = \frac{1}{r^*} \frac{\partial}{\partial r^*}(r^* V^*_r) + \frac{\partial V^*_z}{\partial z^*}. \tag{38}$$

with

$$q^*_r = \frac{L^2}{\delta^2} \left(\frac{-KT_0}{\eta_0 V_0^2 Re} \frac{\partial T^*}{\partial r^*} \right), \qquad q^*_z = \frac{-KT_0}{\eta_0 V_0^2 Re} \frac{\partial T^*}{\partial z^*}$$

where $Re = \varrho_0 V_0 L / \eta_0$ is the Reynolds number, $\lambda^* = -2\eta^*/3$ and $E^*_t = E_t/(\varrho_0 V_0^2)$.

We write these dimensionless equations in the weak conservative form

$$\frac{\partial U^*}{\partial t^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*}(r^* G^*) + \frac{\partial F^*}{\partial z^*} + \frac{1}{r^*} H^* = 0 \tag{39}$$

where

$$U^* = \begin{bmatrix} \varrho^* \\ \varrho^* V^*_r \\ \varrho^* V^*_z \\ E^*_t \end{bmatrix}, \quad G^* = \begin{bmatrix} \varrho^* V^*_r \\ \varrho^* V^*_r V^*_r + \frac{L^2}{\delta^2} P^* - \frac{L^2}{\delta^2} \tau^*_{rr}/Re \\ \varrho^* V^*_r V^*_z - \frac{L^2}{\delta^2} \tau^*_{rz}/Re \\ (E^*_t + P^*) V^*_r - V^*_r \tau^*_{rr}/Re - \frac{L^2}{\delta^2} V^*_z \tau^*_{rz}/Re + q^*_r \end{bmatrix} \tag{40}$$

$$F^* = \begin{bmatrix} \varrho^* V^*_z \\ \varrho^* V^*_r V^*_z - \frac{L^2}{\delta^2} \tau^*_{rz}/Re \\ \varrho^* V^*_z V^*_z + P^* - \tau^*_{zz}/Re \\ (E^*_t + P^*) V^*_z - V^*_r \tau^*_{rz}/Re - V^*_z \tau^*_{zz}/Re + q^*_z \end{bmatrix}, \quad H^* = \begin{bmatrix} 0 \\ -\frac{L^2}{\delta^2} P^* + \frac{L^2}{\delta^2} \tau_{\theta\theta}/Re \\ 0 \\ 0 \end{bmatrix}. \tag{41}$$

The solution domain is now $0 \le r^* \le f(Lz^*)/\delta$ and $0 \le z^* \le b/L$.

The change of variable

$$x = \frac{z^*}{b/L}, \qquad y = \frac{r^*}{f(Lz^*)/\delta} \tag{42}$$

converts the system of equations (39) to the form

$$\frac{\partial U}{\partial t^*} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + H = 0 \tag{43}$$

over the domain $0 \leq x \leq 1$ and $0 \leq y \leq 1$ where

$$\begin{aligned} E &= \frac{L}{b} F^*, \quad F = \frac{\delta}{f(bx)} G^* - \frac{Lyf'(bx)}{f(bx)} F^*, \\ H &= \frac{Lf'(bx)}{f(bx)} F^* + \frac{\delta}{yf(bx)} (G^* + H^*), \quad U = U^* \end{aligned} \tag{44}$$

Note that in the limit as $y \to 0$ we have the result

$$\lim_{y \to 0} \frac{G^* + H^*}{y} = \begin{bmatrix} \varrho^* \frac{\partial V_r^*}{\partial y} \\ 0 \\ \varrho^* V_z^* \frac{\partial V_r^*}{\partial y} - \frac{L^2}{\delta^2} \frac{1}{Re} \frac{\partial \tau_{rz}^*}{\partial y} \\ (E_t^* + P^*) \frac{\partial V_r^*}{\partial y} - \frac{\tau_{rr}^*}{Re} \frac{\partial V_r^*}{\partial y} - \frac{L^2}{\delta^2} \frac{1}{Re} (V_z^* \frac{\partial \tau_{rz}}{\partial y} + \tau_{rz}^* \frac{\partial V_z^*}{\partial y}) + \frac{\partial q_r^*}{\partial y} \end{bmatrix} \tag{45}$$

Using the vector of primitive variables

$$V = \text{Col}(\varrho^*, V_r^*, V_z^*, T^*) \tag{46}$$

and the vector of computational variables

$$U = \text{Col}(\varrho^*, \varrho^* V_r^*, \varrho^* V_z^*, E_t^*) \tag{47}$$

we obtain the first three primitive variables from the computational variables from the relations

$$V_1 = U_1 = \varrho^* \tag{48}$$

$$V_2 = U_2 / U_1 = V_r^* \tag{49}$$

$$V_3 = U_3 / U_1 = V_z^*. \tag{50}$$

The remaining primitive variable is determined using Newton's iterative method on the system

$$T_{n+1} = T_n - \frac{e(T_n) - e_0}{C_v(T_n)} \tag{51}$$

where $e_0 = V_0^2 (U_4 - \frac{1}{2} V_1 (\frac{\delta^2}{L^2} V_2^2 + V_3^2)) / V_1$ and $e(T)$ is given by equation (9) with $\frac{\partial e}{\partial T} = C_v$. After solving for T we calculate $V_4 = T^* = T/T_0$. Conversely, we can construct the computational variables from the primitive variables using the relations

$$\begin{aligned} U_1 &= V_1 \\ U_2 &= V_1 * V_2 \\ U_3 &= V_1 * V_3 \\ U_4 &= V_1 * e(T_0 * V_4) + V_1 * (\frac{\delta^2}{L^2} V_2^2 + V_3^2)/2. \end{aligned} \tag{52}$$

Operator Splitting

The weak conservative form for the equations of motion in terms of the computational coordinates x, y are given by the system of equations (43). We can then define the operator L_x as the numerical solution of the system $\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} = 0$ given by

$$\begin{aligned} \text{Predictor:} \quad & U_{i,j}^{\overline{**}} = U_{i,j}^{*} - \frac{\Delta t}{\Delta x}(E_{i+1,j}^{*} - E_{i,j}^{*}) \\ \text{Corrector:} \quad & U_{i,j}^{**} = \frac{1}{2}(U_{i,j}^{*} + U_{i,j}^{\overline{**}} - \frac{\Delta t}{\Delta x}(E_{i,j}^{\overline{**}} - E_{i-1,j}^{\overline{**}})). \end{aligned}$$

Define the operator L_y as the numerical solution of the system $\frac{\partial U}{\partial t} + \frac{\partial F}{\partial y} = 0$

$$\begin{aligned} \text{Predictor:} \quad & U_{i,j}^{\overline{**}} = U_{i,j}^{*} - \frac{\Delta t}{\Delta y}(F_{i,j+1}^{*} - F_{i,j}^{*}) \\ \text{Corrector:} \quad & U_{i,j}^{**} = \frac{1}{2}(U_{i,j}^{*} + U_{i,j}^{\overline{**}} - \frac{\Delta t}{\Delta y}(F_{i,j}^{\overline{**}} - F_{i,j-1}^{\overline{**}})). \end{aligned}$$

Define the operator L as the numerical solution of the system $\frac{\partial U}{\partial t} + H = 0$ as

$$\begin{aligned} \text{Predictor:} \quad & U_{i,j}^{\overline{**}} = U_{i,j}^{*} - \Delta t H_{i,j}^{*} \\ \text{Corrector:} \quad & U_{i,j}^{**} = \frac{1}{2}(U_{i,j}^{*} + U_{i,j}^{\overline{**}} - \Delta t H_{i,j}^{\overline{**}}) \end{aligned}$$

where $F_{i,j}^{*} = F(U_{i,j}^{*}), H_{i,j}^{\overline{**}} = H(U_{i,j}^{\overline{**}})$, etc.

For the method of operator splitting we time march according to the sequence of operators

$$U_{i,j}^{n+2} = L_x\, L_y\, L\, L\, L_y\, L_x\, U_{i,j}^{n}$$

and progress the solution from time $n\Delta t^*$ to $(n+2)\Delta t^*$ where Δt^* is selected to satisfy the Courant-Fredrich-Lewy CFL stability condition. The CFL stability condition is determined by time steps Δt_z and Δt_r evaluated at all internal node points. These time steps are given by (reference [7])

$$\Delta t_z = \frac{b h_1}{|V_z| + \sqrt{\gamma R T} + \frac{1}{\varrho}\left(\frac{2\gamma K}{b h_1 C_p} + \frac{\sqrt{2\eta^2/3}}{f(bx)k_1}\right)}$$

$$\Delta t_r = \frac{f(bx)k_1}{|V_r| + \sqrt{\gamma R T} + \frac{1}{\varrho}\left(\frac{2\gamma K}{f(bx)k_1 C_p} + \frac{\sqrt{2\eta^2/3}}{b h_1}\right)}.$$

From all such time steps we select the minimum time step $\Delta t = \underset{\text{all i,j}}{\text{Min}}\{\Delta t_z, \Delta t_r\}$ and then scale this real time to calculate the scaled time step $\Delta t^* = \frac{\Delta t V_0}{L}$.

Other methods to solve the system of equations (43) are Runge-Kutta methods and various implicit methods. Current research is trying to establish an efficient method for solving the system of equations (43) together with appropriate boundary conditions.

Two Temperature Model

For our second model we assume a vibrational degree of freedom together with a combined rotational-translational degree of freedom. Each degree of freedom is assumed to follow a Boltzmann distribution and the energy content of each degree of freedom is characterized by temperatures T_v and T respectively. As the gas passes through the nozzle there is a certain finite relaxation time τ for the vibrational mode of excitation to achieve equilibrium with the rotational-translational mode of excitation. Define the quantities:

n_i Population density of ith energy level

ϵ_i Energy per molecule of the ith level

$\dot{n}_i$ Time rate of change of n_i due to collisions

$\vec{q}_t$ Heat flux

$\vec{q} = \vec{q}_{rr} + \vec{q}^*$

where $\vec{q}_{rr}$ is the heat flux due to rotational energy

$\vec{q}^*$ Heat flux due to energy excitation of all energy levels

*Total energy from all energy levels

$$\vec{q}^* = \sum_i n_i \epsilon_i \vec{U}_i$$

where $\vec{U}_i = \vec{V}_i - \vec{V}$ is the diffusion velocity of molecule in state i

Φ The Dissipation function.

Let $\varrho e^* = \sum_i n_i \epsilon_i$ denote the total energy per unit volume of the vibrational mode so that by integrating over the volume and surface of an arbitrary volume element we obtain

$$\frac{d}{dt}\int_V \varrho e^* \, dv = -\int_S \sum_i n_i \epsilon_i \vec{V}_i \cdot d\vec{S} + \int_V \sum_i \dot{n}_i \epsilon_i \, dv$$

where dv is a volume element and $d\vec{S}$ is an area element of the control volume and $\dot{n}_i$ are rate equations to be determined. Using the Gauss divergence theorem and interchanging the order of summation and integration there results

$$\begin{aligned} \frac{\partial}{\partial t}(\varrho e^*) + \sum_i \nabla(n_i \epsilon_i(\vec{U}_i + \vec{V})) &= \sum_i \dot{n}_i \epsilon_i \\ \frac{\partial}{\partial t}(\varrho e^*) + \nabla(\varrho e^* \vec{V}) &= \sum_i \left[\dot{n}_i \epsilon_i - \nabla(n_i \epsilon_i \vec{U}_i)\right]. \end{aligned} \tag{53}$$

Using the identities

$$\frac{D}{Dt}(\varrho e^*) = \frac{\partial(\varrho e^*)}{\partial t} + \vec{V}\cdot\nabla(\varrho e^*) + \nabla(\varrho e^* \vec{V}) - \varrho e^* \nabla\cdot\vec{V} - \vec{V}\cdot\nabla(\varrho e^*)$$

together with the continuity equation and

$$\frac{D}{Dt}(\varrho e^*) = \varrho\frac{De^*}{Dt} + e^*\frac{D\varrho}{Dt} = \varrho\frac{De^*}{Dt} - \varrho e^*\nabla\cdot\vec{V}$$

we write the vibrational energy equation as

$$\varrho\frac{De^*}{Dt} = \sum_i \dot{n}_i\epsilon_i - \nabla\vec{q}^*.$$

Assuming linear harmonic oscillators and using the rate equations from Meador, et. al., reference [5],

$$\frac{1}{\varrho}\sum_i \dot{n}_i\epsilon_i = \frac{e_e^* - e^*}{\tau}$$

where the subscript e denotes equilibrium, the above equation becomes

$$\frac{De^*}{Dt} = \frac{e_e^* - e^*}{\tau} - \frac{1}{\varrho}\nabla\cdot\vec{q}^*.$$

Letting $*$ denote the vibrational mode then if T_v exists, the vibrational energy equation can be represented as

$$\varrho\frac{De_v}{Dt} \equiv \varrho C_{vv}\frac{DT_v}{Dt} = \varrho\left[\frac{e_v(T) - e_v(T_v)}{\tau}\right] - \nabla\cdot\vec{q}_v. \tag{54}$$

The second energy equation is obtained by substituting $e = e_{rt} + e_v$ into the energy equation (4) to obtain the form

$$\varrho\frac{\partial}{\partial t}(e_{rt}+e_v) + \varrho\vec{V}\cdot\nabla(e_{rt}+e_v) + P\nabla\cdot\vec{V} + \nabla(\vec{q}_{rt}+\vec{q}_v) - \Phi + \varrho C_{vv}X - \varrho C_{vv}X = 0 \tag{55}$$

where

$$C_{vv}X = \frac{e_v(T) - e_v(T_v)}{\tau} \tag{56}$$

and then employing the vibrational equation (54) to obtain the coupled energy equations

$$\begin{aligned} \varrho\frac{\partial e_{rt}}{\partial t} + \varrho\vec{V}\cdot\nabla e_{rt} + P\nabla\cdot\vec{V} + \nabla\cdot\vec{q}_{rt} - \Phi + \varrho C_{vv}X &= 0 \\ \varrho\frac{\partial e_v}{\partial t} + \varrho\vec{V}\cdot\nabla e_v + \nabla\cdot\vec{q}_v - \varrho C_{vv}X &= 0 \end{aligned} \tag{57}$$

which reduce to the form

$$\begin{aligned} \frac{DT}{Dt} &= \frac{-1}{\varrho C_{rt}}\left(\nabla\cdot\vec{q}_{rt} - \Phi + P\nabla\cdot\vec{V} + \varrho C_{vv}X\right) \\ \frac{DT_v}{Dt} &= \frac{-1}{\varrho C_{vv}}\nabla\cdot\vec{q}_v + X \end{aligned} \tag{58}$$

where

$$e_v(T) = \int_{T_v}^{T} C_{vv}\, dT = \int_{T_v}^{T} R\left(\frac{\phi}{T}\right)^2 \frac{e^{\phi/T}}{(e^{\phi/T}-1)^2}\, dT. \tag{59}$$

The integral in equation (59) is used to calculate the quantity

$$X = \frac{1}{C_{vv}\tau}(e_v(T) - e_v(T_v)).$$

Integration produces the result

$$X = \frac{T_v^2}{\phi\tau}\frac{1-e^{-\phi/T_v}}{1-e^{-\phi/T}}\left\{\exp\left[\phi\left(\frac{1}{T_v}-\frac{1}{T}\right)\right]-1\right\}. \tag{60}$$

The quantity $\varrho C_{vv}X = \frac{\varrho}{\tau}(e_v(T) - e_v(T_v))$ can be viewed as a coupling term for energy between the vibrational and rotational-translational modes. The other terms in the coupled equations (43) are given by

$$C_v = C_{vrt} + C_{vv}, \qquad C_{vrt} = 5R/2, \qquad C_{vv} = R(\phi/T_v)^2\frac{e^{\phi/T_v}}{(e^{\phi/T_v}-1)^2} \tag{61}$$

$$e_{rt} = \frac{5}{2}RT \tag{62}$$

$$e_v = \int_{T_0}^{T_v} C_{vv}\, dT = \frac{R\phi}{e^{\phi/T_v}-1} - \frac{R\phi}{e^{\phi/T_0}-1} \tag{63}$$

$$X = \frac{1}{C_{vv}\tau}(e_v(T) - e_v(T_v))$$

$$X = \frac{T_v^2}{\phi\tau}\left(\frac{1-e^{-\phi/T_v}}{1-e^{-\phi/T}}\right)\left\{\exp\left[\phi\left(\frac{1}{T_v}-\frac{1}{T}\right)\right]-1\right\} \tag{64}$$

$$\vec{q_{rt}} = -K_{rt}\nabla T \tag{65}$$

$$\vec{q_v} = -K_v\nabla T_v \tag{66}$$

$$K_{rt} = 4.93\eta R \tag{67}$$

$$K_v = 1.35\eta C_{vv} \tag{68}$$

$$\eta = \frac{c_1 g_c T^{3/2}}{T + c_2} \quad \text{Sutherland's formula} \tag{69}$$

$$c_1 = (1.488) * 2.16(10^{-8}), \quad g_c = 32.174, \quad c_2 = 184.0 \tag{70}$$

Here we have assumed that the coefficient for self diffusion between molecules in different internal states is a constant for all energy states. This in turn produces the above specific heats.

The divergence of the heat flux terms are given by

$$\nabla\cdot\vec{q}_{rt} = -K_{rt}\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) - \frac{\partial K_{rt}}{\partial T}\left[\left(\frac{\partial T}{\partial r}\right)^2 + \left(\frac{\partial T}{\partial z}\right)^2\right] \tag{71}$$

$$\nabla\cdot\vec{q}_v = -K_v\left(\frac{\partial^2 T_v}{\partial r^2} + \frac{1}{r}\frac{\partial T_v}{\partial r} + \frac{\partial^2 T_v}{\partial z^2}\right) - \frac{\partial K_v}{\partial T_v}\left[\left(\frac{\partial T_v}{\partial r}\right)^2 + \left(\frac{\partial T_v}{\partial z}\right)^2\right]. \tag{72}$$

For the pressure we assume an equation of state for an ideal gas $P = \rho RT$. Following Meador et.al. [5] the relaxation time τ for N_2 is taken as

$$P(atm)\tau = \frac{3.2188(10^{-12})}{I(T)\sinh(\phi/2T)}\left(\frac{T}{\theta}\right)^{1/2}\exp(-\xi/T) \tag{73}$$

where ϕ, θ, ξ are characteristic temperatures given by $\phi = 3395\,K$, $\theta = 3.2324(10^7)\,K$, $\xi = 95.9\,K$, and

$$I(T) = \int_{\frac{\phi+2\xi}{2T}}^{\infty}\left[1+\left(1+\frac{Tx}{\xi}\right)^{1/2}\right]^{-1/3}(1-e^{-2\zeta_-})\exp[-(x+\zeta_+-\zeta_-)]\,dx \tag{74}$$

where

$$\zeta_\pm = \left[\frac{16\theta Tx}{27\phi^2}\left(1\pm\frac{\phi}{2Tx}\right)\right]^{1/2}. \tag{75}$$

For the two temperature model we replace the single temperature equation by two temperature equations. We define the column vector of primitive variables

$$V = \mathrm{col}(\,\varrho,\, V_r,\, V_z,\, T,\, T_v) \tag{76}$$

and use the computational variables

$$U = \mathrm{Col}(\,\varrho,\, \varrho V_r,\, \varrho V_z,\, E_{rt},\, E_v). \tag{77}$$

This requires that we replace the temperature equations (58) by energy equations in conservative form. The conservative form of the split energy equations are obtained by substituting $E_t = E_{rt} + E_v$ into the equation (18) to obtain the equations

$$\begin{aligned}
\frac{\partial E_{rt}}{\partial t} &+ \frac{1}{r}\frac{\partial}{\partial r}(r[(E_{rt}+P)V_r - V_r\tau_{rr} - V_z\tau_{rz} + q_{rt}]) \\
&+ \frac{\partial}{\partial z}[(E_{rt}+P)V_z - V_r\tau_{rz} - V_z\tau_{zz} + q_{zrt}] + \varrho C_{vv}X = 0 \\
\frac{\partial E_v}{\partial t} &+ \frac{1}{r}\frac{\partial}{\partial r}[r(E_v V_r + q_{rv})] + \frac{\partial}{\partial z}[E_v V_z + q_{zv}] - \varrho C_{vv}X = 0
\end{aligned}$$

where

$$\begin{aligned}
E_{rt} &= \varrho e_{rt} \qquad & E_{rt} &= \frac{5}{2}\varrho RT + \frac{\varrho}{2}(V_r^2 + V_z^2) \\
E_v &= \varrho e_v \qquad & E_v &= \varrho R\phi/(e^{\phi/T_v} - 1)
\end{aligned}$$

These equations must be scaled and added to the continuity and momentum equations developed earlier. The resulting set of coupled equations are given by

$$\frac{\partial U^*}{\partial t^*} + \frac{1}{r^*}\frac{\partial}{\partial r^*}(r^* G^*) + \frac{\partial F^*}{\partial z^*} + \frac{1}{r^*}H^* = 0$$

where

$$U^* = \begin{bmatrix} \varrho^* \\ \varrho^* V_r^* \\ \varrho^* V_z^* \\ E_{rt}^* \\ E_v^* \end{bmatrix}, \quad G^* = \begin{bmatrix} \varrho^* V_r^* \\ \varrho^* V_r^* V_r^* + \frac{L^2}{\delta^2} P^* - \frac{L^2}{\delta^2} \tau_{rr}^* / Re \\ \varrho^* V_r^* V_z^* - \frac{L^2}{\delta^2} \tau_{rz}^* / Re \\ (E_{rt}^* + P^*) V_r^* - V_r^* \tau_{rr}^* / Re - \frac{L^2}{\delta^2} V_z^* \tau_{rz}^* / Re + q_{rt}^* \\ E_v^* V_r^* + q_{rv}^* \end{bmatrix}$$

$$F^* = \begin{bmatrix} \varrho^* V_z^* \\ \varrho^* V_r^* V_z^* - \frac{L^2}{\delta^2} \tau_{rz}^* / Re \\ \varrho^* V_z^* V_z^* + P^* - \tau_{zz}^* / Re \\ (E_{rt}^* + P^*) V_z^* - V_r^* \tau_{rz}^* / Re - V_z^* \tau_{zz}^* / Re + q_{zrt}^* \\ E_v^* V_z^* + q_{zv}^* \end{bmatrix}, \quad H^* = \begin{bmatrix} 0 \\ -P^* + \frac{L^2}{\delta^2} \tau_{\theta\theta} / Re \\ 0 \\ r^* Q^* \\ -r^* Q^* \end{bmatrix}.$$

where

$$E_{rt}^* = \frac{E_{rt}}{\varrho_0 V_0^2}, \qquad E_v^* = \frac{E_v}{\varrho_0 V_0^2}, \qquad T_v^* = \frac{T_v}{T_0}$$

$$q_{rt}^* = \frac{L}{\delta} \frac{q_{rt}}{\varrho_0 V_0^3}, \qquad q_{zrt}^* = \frac{q_{zrt}}{\varrho_0 V_0^3}$$

$$q_{rv}^* = \frac{L}{\delta} \frac{q_{rv}}{\varrho_0 V_0^3}, \qquad q_{zv}^* = \frac{q_{zv}}{\varrho_0 V_0^3}$$

$$Q^* = \frac{L \varrho^* C_{vv}^* X^*}{V_0^3},$$

$$C_{vv}^* = C_{vv}|_{T = T_0 T^*}, \qquad X^* = X|_{\substack{T_v = T_0 T_v^* \\ T = T_0 T^*}}$$

The above equations involve the primitive variables

$$V = \mathrm{Col}(\varrho, V_r, V_z, T, T_v)$$

and conservative variables

$$U = \mathrm{Col}(\varrho, \varrho V_r, \varrho V_z, E_{rt}, E_v).$$

Boundary Conditions

The initial inlet temperature, inlet pressure, and inlet density, are given a priori. From these values we calculate the critical values $V^*, P^*, \varrho^*, A^*, T^*$ from a one dimensional model for the flow and from these values determine the inlet velocity. The one dimensional nozzle values of pressure, temperature, density and velocity are calculated as a function of nozzle distance z. These values are then used as starting values for each model. We require a no slip boundary condition at the nozzle walls, symmetry with respect to the centerline, and normal derivative of the pressure to be zero at the walls. Extrapolated boundary conditions are then applied to the exit values and as well as extrapolated temperature values at the wall and centerline. The exit pressure is also initially assigned.

Comparison with isentropic one-dimensional model

For comparison purposes we also assume an isentropic process and calculate the results for a one-dimensional flow through the nozzle in the z direction where the area of the nozzle is a function of z. For an isentropic process we have

$$ds = \frac{dh - \frac{dP}{\varrho}}{T} = 0,$$

with $h = e + RT$, $e = \int_{T_0}^{T} C_v(T)\,dT$ and $dh = C_p\,dT$. Consequently,

$$ds = C_p\,\frac{dT}{T} - R\frac{dP}{P} = 0 \tag{78}$$

or

$$\int_{P_0}^{P} \frac{dP}{P} = \int_{T_0}^{T} \left[\frac{7}{2} + \left(\frac{\phi}{T}\right)^2 \frac{e^{\phi/T}}{(e^{\phi/T}-1)^2}\right] \frac{dT}{T}. \tag{79}$$

Let

$$V = \frac{1}{e^{\phi/T}-1}, \qquad dV = \frac{e^{\phi/T}}{(e^{\phi/T}-1)^2}\frac{\phi}{T^2}\,dT \tag{80}$$

and integrate by parts to obtain

$$\log P\,|_{P_0}^{P} = \frac{7}{2}\log T\,|_{T_0}^{T} + \frac{\phi}{T}\frac{1}{e^{\phi/T}-1}\,|_{T_0}^{T} + \int_{T_0}^{T} \frac{\phi}{T^2}\frac{1}{e^{\phi/T}-1}\,dT. \tag{81}$$

In the last integral, let $z = e^{\phi/T} - 1$,$dz = -e^{\phi/T}\frac{\phi}{T^2}dT$ so that

$$\int_{T_0}^{T} \frac{\phi}{T^2}\frac{1}{e^{\phi/T}-1}\,dT = -\int_{z_0}^{z} \frac{dz}{z(z+1)} = -\int_{z_0}^{z}\frac{dz}{z} + \int_{z_0}^{z}\frac{dz}{z+1}$$

and consequently

$$\int_{T_0}^{T} \frac{\phi}{T^2}\frac{1}{e^{\phi/T}-1}\,dT = \log\left(\frac{1-e^{-\phi/T_0}}{1-e^{-\phi/T}}\right). \tag{82}$$

Therefore, we can calculate the pressure ratio as

$$\frac{P}{P_0} = \left(\frac{T}{T_0}\right)^{7/2} \left(\frac{1 - e^{-\phi/T_0}}{1 - e^{-\phi/T}}\right) \exp\left(\frac{\phi/T}{e^{\phi/T} - 1} - \frac{\phi/T_0}{e^{\phi/T_0} - 1}\right). \tag{83}$$

Since $P = \varrho RT$ we can write

$$\frac{\varrho}{\varrho_0} = \left(\frac{T}{\phi}\frac{\phi}{T_0}\right)^{5/2} \left(\frac{1 - e^{-\phi/T_0}}{1 - e^{-\phi/T}}\right) \exp\left(\frac{\phi/T}{e^{\phi/T} - 1} - \frac{\phi/T_0}{e^{\phi/T_0} - 1}\right). \tag{84}$$

where ϕ/T_0 is treated as a parameter.

In one dimension the energy equation can be written

$$dh + V_z\,dV_z = 0 \quad \text{or} \quad C_p\,dT + V_z\,dV_z = 0. \tag{85}$$

Consequently, we may write

$$\int_{V_{z_0}}^{V_z} V_z\,dV_z = -\int_{T_0}^{T} C_p\,dT$$

which integrates to

$$V_z^2 - V_{z_0}^2 = 7R(T_0 - T) + 2R\phi\left(\frac{1}{e^{\phi/T_0} - 1} - \frac{1}{e^{\phi/T} - 1}\right). \tag{86}$$

By dividing by $a^2 = \gamma RT$, the local speed of sound, the one dimensional mach number can be represented

$$M^2 = \frac{V_{z_0}^2}{\gamma RT} + \frac{7}{\gamma}\left(\frac{T_0}{T} - 1\right) + \frac{2\phi}{\gamma T}\left(\frac{1}{e^{\phi/T_0} - 1} - \frac{1}{e^{\phi/T} - 1}\right) \tag{87}$$

with $M = V_z/a$. The mach number and one dimensional analysis is used to obtain an approximate solution to the more complicated two dimensional problem. Here

$$\gamma = \frac{C_p}{C_v} = \frac{7 + 2(\phi/T)^2 e^{\phi/T}(e^{\phi/T} - 1)^{-2}}{5 + 2(\phi/T)^2 e^{\phi/T}(e^{\phi/T} - 1)^{-2}}. \tag{88}$$

The one dimensional continuity equation is given by

$$AV_z\varrho = A^* V_z^* \varrho^* \tag{89}$$

where the $*$ quantities represent those values at the throat of the nozzle where $M = 1$. That is, set $M = 1$ in equation (84), then solve the equations (84)(85) simultaneously for the value of ϕ/T, treating ϕ/T_0 as a parameter. This calculated value of ϕ/T gives $T = T^*$ when $M = 1$ and consequently we can calculate the values of $P^*, \varrho^*, \gamma^*, V_z^* = \gamma^* RT^*$ at this critical value of the temperature. The equation (86) can then be expressed in the following form involving the above critical parameters

$$
\begin{aligned}
\frac{A}{A^*} &= \frac{V_z^* \varrho^*}{V_z \varrho} = \frac{\frac{V_z^*}{\sqrt{\gamma^* R T^*}}}{\frac{V_z}{\sqrt{\gamma R T}} \frac{\sqrt{\gamma R T}}{\sqrt{\gamma^* R T^*}}} \frac{R \varrho^* T^*}{R \varrho T \frac{T^*}{T}} \\
\frac{A}{A^*} &= \frac{1}{M} \sqrt{\frac{\gamma^* T^*}{\gamma T} \frac{P^*}{P \frac{T^*}{T}}} = \frac{1}{M} \sqrt{\frac{\gamma^* T}{\gamma T^*} \frac{P^*}{P}} \\
\frac{A}{A^*} &= \frac{1}{M} \sqrt{\frac{\gamma^*}{\gamma} \frac{T}{\phi} \frac{\phi}{T^*} \frac{P^*}{P_0} \frac{P_0}{P}}.
\end{aligned} \tag{90}
$$

Knowing the critical values T^*, γ^*, P^*, A^* we can calculate the ratio T/ϕ as a function of A/A^* which is a function of z, with T_0/ϕ as a parameter. These one dimensional values are then used as starting values for the solution of the two dimensional non-isentropic nozzle problem.

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APPENDIX A
LIST OF SYMBOLS

a	Speed of Sound $[m/s]$
A	Cross sectional area $[m^2]$
$\vec{b}$	Body force per unit mass $[Newton/Kg]$
C_v, C_{vrt}, C_{vv}	Specific heat at constant volume $[Joule/Kg\,K]$
$D_{i,j}$	Rate of deformation tensor $[s^{-1}]$
$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{V} \cdot \nabla$	Material or substantial derivative
e, e_{rt}, e_v	Energy per unit mass $[Joule/Kg]$
E_{rt}, E_v, E_t	Energy per unit volume $[Joule/m^3]$
$\hbar$	Planck's constant $[Joule\,s]$
h	Enthalpy $[Joule/m^3]$
k	Boltzmann's constant $[Joule/K]$
K, K_{rt}, K_v	Thermal conductivities $[W/m\,K]$
$m = W/N_a$	Molecular mass $[Kg]$
M	Mach number
N_a	Avogadro's number $[mol^{-1}]$
$\vec{q}, \vec{q}_{rt}, \vec{q}_v$	Energy flux $[Joule/m^2\,s]$
P	Pressure $[Newton/m^2]$
Q	External heat source per unit volume $[Joule/m^3]$
R	Gas Constant $[Joule/Kg\,K]$
r	Radial distance $[m]$
s	Entropy per unit volume $[Joule/m^3\,K]$
t	Time $[s]$
T, T_v	Temperatures $[K]$

$\vec{V}$	Velocity $[m/s]$
V_r, V_z	Velocity components $[m/s]$
W	Molecular weight of N_2 $[Kg/mol]$
X	Coupling term $[K/s]$
x, y	Computational coordinates
z	axial distance $[m]$
η	Viscosity coefficient $[Kg/m\,s]$
λ	Second coefficient of viscosity $[Kg/m\,s]$
ϱ	Density $[Kg/m^3]$
τ	Relaxation time $[s]$
τ_{ij}	Stress tensor $[Newton/m^2]$
ϕ, θ, ξ	Characteristic temperatures $[K]$
ν	Frequency $[s^{-1}]$
$\gamma = \frac{C_p}{C_v}$	Ratio of specific heats
Φ	Dissipation function $[Joule/m^3\,s]$