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Numerical Simulation of Fluid Dynamics and Payload Dissemination in a Dual-Chamber Grenade

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1. INTRODUCTION

The dissemination of solid payload material as a gaseous cloud from a container can be accomplished using a pressurized system (e.g. compressed CO₂ cartridge), a mechanical system (e.g. plunger) or a pyrotechnic system (e.g. central burster or hot/cold gas flow). In the latter technique, dissemination of the payload is realized after ablation and vaporization of the material from exposure to the thermal effects of pyrotechnic combustion. Experimental programs at the U.S. Army Chemical Research Development and Engineering Center (CRDEC) are being used to test the efficiency of the thermal/ablation method. The goals are high rate of dissemination and low temperature/high payload concentration in the dissemination cloud. These tests can involve highly instrumented full-scale and small-scale grenade models ignited within large test chambers. Numerical simulation in support of such tests was conducted at the U.S. Army Research Laboratory (ARL). These simulations are required to aid in data reduction, contribute to the physical understanding of thermal dissemination, and conduct parametric studies that may guide future tests.

The internal design of a grenade used for the thermal dissemination of solid payload into the atmosphere can consist of two concentric cylinders; a pyrotechnic device in the outer annulus and payload material bonded to the wall of the inner cylinder. The two chambers are connected. Combustion of the pyrotechnic produces a high pressure within the grenade. A pressure difference between the atmosphere and inside the grenade induces a thru-flow that thermally erodes and vaporizes the material in the inner chamber. The material in gaseous form is entrained in this flow and expelled from the grenade. Figure 1 shows the internal schematic of a generic grenade configuration.

Numerical simulation of the fluid dynamics associated with payload dissemination from a grenade is accomplished in the present study using the Navier-Stokes equations along with equations that govern chemical species ablation and diffusion. Chemical reactions between payload and pyrotechnic gases may be but are not necessarily involved. An implicit finite-difference scheme based on successive-over-relaxation is used to solve these equations for the physical domain of interest. This domain resides within the inner chamber of the grenade; thus, the flow within the grenade is modeled excluding combustion of the pyrotechnic. Using chamber dimensions and payload chemical properties this simulation yields velocity, pressure, temperature, density and chemical composition of the gas in the inner chamber and exiting the grenade.

2. NUMERICAL SIMULATION

The RAMCOMB (RAMjet COMBustion) computer code was originally developed for the numerical simulation of combustion in a tubular solid-fuel ramjet (SFRJ) projectile (Nusca et.al. 1988, Nusca 1989). Solid fuel regression rate and projectile thrust predictions compared favorably with in-flight and ground test data. For the SFRJ application the RAMCOMB code simulated a mass-controlled (stoichiometric) reaction of non-premixed solid fuel and oxygen using classical diffusion flame techniques. The code has also been used to simulate finite-rate premixed gaseous fuel combustion in the ram accelerator projectile launch system (Nusca 1991) with reaction rates formulated in terms of temperature and chemical species mass fraction. Application of the code to payload dissemination simulation for grenades involves chemical species ablation and diffusion without chemical reactions. The governing equations, boundary and initial conditions as well as the solution method are outlined below.

2.1 Governing Equations. Since the grenade payload chamber geometry is axisymmetric (Fig. 1) the governing equations can be written in cylindrical coordinates. The velocity components in this system are u, v , and w for the radial (r), azimuthal (θ), and axial (z) directions, respectively. Axisymmetric flow is assumed thus, all θ -derivatives are ignored; however, the azimuthal velocity component and the azimuthal momentum equation are retained (for future consideration of chamber rotation). Since steady flows are considered, time derivatives ($\partial/\partial t$) are ignored. The conservation equations for global mass, momentum (radial, axial, azimuthal) and species mass conservation are given by (Nusca 1991, Schlichting 1979),

$$\nabla \cdot \rho \vec{V} = \frac{1}{r} \frac{\partial(r\rho u)}{\partial r} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (1)$$

$$\nabla \cdot [\rho u \vec{V} - \vec{\tau}_r] - \frac{1}{r} [\rho v^2 - \tau_{\theta\theta}] + \frac{\partial p}{\partial r} = 0 \quad (2)$$

$$\nabla \cdot [\rho w \vec{V} - \vec{\tau}_z] + \frac{\partial p}{\partial z} = 0 \quad (3)$$

$$\frac{1}{r} \nabla \cdot [r(\rho v \vec{V} - \vec{\tau}_\theta)] = 0 \quad (4)$$

$$\frac{1}{r} \left[\frac{\partial}{\partial r} (r\rho u m_j + rJ_{j,r}) + \frac{\partial}{\partial z} (r\rho w m_j + rJ_{j,z}) \right] = 0 \quad (5)$$

Energy conservation for a compressible flow is expressed by the First Law of Thermodynamics. The steady form of the First Law states that the net rate of stagnation enthalpy ($\tilde{h} = h + V^2/2$) inflow for a control volume is equal to the sum of the shear work done by the contents of the control volume on the surroundings ($\vec{\tau}$) and the heat transfer to the

surroundings (Schlichting 1979).

$$\nabla \cdot \left[\rho \vec{V} \vec{h} + \vec{J}_h + \sum_{j=1}^N h_j \vec{J}_j + \vec{J}_k - (u \vec{\tau}_r + v \vec{\tau}_\theta + w \vec{\tau}_z) \right] = 0 \quad (6)$$

where \vec{J} is a flux term for mass ($\vec{J}_j = (\mu_{eff}/Re) \nabla m_j = \Gamma_j \nabla m_j$), heat ($\vec{J}_h = (\mu_{eff}/Pr) c_p \nabla T = \Gamma_h c_p \nabla T$), and turbulence kinetic energy, k , ($\vec{J}_k = (\mu_{eff}/Pr) \nabla k = \Gamma_k \nabla k$). Where Γ represents the diffusion coefficient. The mass fraction and molar specific enthalpy for species j are m_j and h_j , respectively. The density, pressure, velocity vector and velocity magnitude are given by $\rho, p, \vec{V}, V = \sqrt{u^2 + v^2 + w^2}$, respectively.

In Equations 2-4,6 the shear stress ($\vec{\tau}$) includes the Reynolds stress with an effective fluid viscosity expressed as the sum of the molecular and turbulent viscosities, $\mu_{eff} = \mu + \mu_t$. The flow Reynolds number, Re , represents the ratio of mass flux ($\rho V L$) to fluid viscosity, μ_{eff} . Molecular viscosity (μ) is defined using Sutherland's expression (Ames 1958),

$$\mu = 2.270 \times 10^{-8} \frac{T^{1.5}}{T + 198.6} \quad (7)$$

Turbulent viscosity (μ_t) is described in the next section of this report.

The calorically perfect gas assumption can be used to determine the specific heat of each species, c_p , when the temperature dependence of the species is not well determined. The specific heat can also be formulated using an explicit temperature dependence obtained from tabulated data (Stull and Prophet 1971).

$$c_p / \tilde{R} = A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4 \quad (8)$$

where the mixture specific heat is given by,

$$c_p = \sum_{j=1}^N m_j c_{p,j} \quad (9)$$

Mixture temperature (T) is obtained from the conservation of energy (Eq. 6) expressed in terms of the stagnation enthalpy,

$$\vec{h} = T \sum_{j=1}^N c_{p,j} m_j + \left[1 - \frac{1}{Pr} \right] \frac{V^2}{2} + \left[\frac{1}{Sc} - \frac{1}{Pr} \right] \frac{\tilde{V}^2}{2} + \left[\frac{1}{Sc} - \frac{1}{Pr} \right] \sum_{j=1}^N h_j m_j \quad (10)$$

where \tilde{V} is the magnitude of the turbulent (fluctuating) velocity, \sqrt{k} . The Schmidt number, $Sc = \mu_{eff}/(\rho \Gamma)$, (ratio of momentum transport to mass transport) is assumed to be unity. The Prandtl number, $Pr = c_p \mu_{eff}/\kappa$, (ratio of momentum transport to heat transport) is assumed to be nearly unity (.9) which is considered adequate for gaseous flows (Bradshaw 1981). The thermal conductivity of the gas mixture is denoted κ .

The mixture equation of state for a thermally perfect gas follows from Dalton's Law,

$$p = \rho \bar{\mathfrak{R}} T \sum_{j=1}^N \frac{m_j}{\mathcal{M}_j} \quad (11)$$

where $\bar{\mathfrak{R}} = \mathfrak{R} \sum_j \mathcal{M}_j$, \mathcal{M}_j is the molecular weight of species j , and \mathfrak{R} is the specific gas constant. Equation 11 is used to recover the density from the numerical solution of the governing equations.

The stream function-vorticity form of the governing equations has been widely utilized and facilitates the use of numerically efficient Gauss-Seidel relaxation algorithms. Stream function, ψ , and vorticity, ω are defined using (Schlichting 1979),

$$\frac{\partial \psi}{\partial r} = r \rho \omega, \quad \frac{\partial \psi}{\partial z} = -r \rho u, \quad \omega = \nabla \times \vec{V} = - \left[\frac{\partial}{\partial z} \left(\frac{1}{r \rho} \frac{\partial \psi}{\partial z} \right) + \frac{\partial}{\partial r} \left(\frac{1}{r \rho} \frac{\partial \psi}{\partial r} \right) \right] \quad (12)$$

The governing equations, derived by Nusca (1989), can be expressed in the form of a general variable, ϕ . This variable can represent stream-function, vorticity, azimuthal velocity, stagnation enthalpy, species mass fraction, turbulence kinetic energy, or turbulence dissipation rate.

$$a_\phi \left[\frac{\partial}{\partial z} \left(\phi \frac{\partial \psi}{\partial r} \right) - \frac{\partial}{\partial r} \left(\phi \frac{\partial \psi}{\partial z} \right) \right] - \frac{\partial}{\partial z} \left[b_\phi r \frac{\partial}{\partial z} (c_\phi \phi) \right] - \frac{\partial}{\partial r} \left[b_\phi r \frac{\partial}{\partial r} (c_\phi \phi) \right] + r d_\phi = 0 \quad (13)$$

For example, $\phi = \psi$, $a_\phi = 0$, $b_\phi = 1/(\rho r^2)$, $c_\phi = 1$, $d_\phi = -\omega/r$ (which yields Eq. 12). For N species only $N - 1$ specie equations ($\phi = m_j$) must be solved, since the sum of the mass fractions must equal unity. In effect the global continuity equation (Eq. 1) is the N th specie equation since the summation of all specie equations yields the continuity equation.

The pressure can be recovered from the $\psi - \omega$ form of the equations after a converged solution of Equation 13 is achieved or after each iteration, if pressure variations are expected to have a significant effect on density. The radial and axial momentum equations (Eq. 2 and 3) can be rearranged to yield:

$$\frac{\partial p}{\partial z} = P_1(r, z) \quad \text{and} \quad \frac{\partial p}{\partial r} = P_2(r, z) \quad (14)$$

where P_1 and P_2 are functions of ρ , V and \vec{r} . Along any path from point A to point B in the flowfield, the pressure is given by:

$$p_B - p_A = \int_A^B (P_1 dz + P_2 dr) \quad (15)$$

Since p is a scalar, $p_B - p_A$ should be path independent and therefore, can serve as a consistency check on the converged solution. In most cases a pressure difference is desired to form the pressure coefficient at a point. However, if the pressure at point B is required the pressure at point A is assigned to a known inlet value and integration proceeds from the inlet to point B in the flowfield.

2.2 Turbulence Model. A two-equation turbulence model has been suggested by Kim and Chung (1989) for multiple species flows. This model describes the turbulence viscosity (μ_t) as a function of turbulence kinetic energy (k) and dissipation rate (ϵ) as $\mu_t = \rho C_3 k^2 / \epsilon$. A set of partial differential equations is written for k and ϵ .

$$\rho w \frac{\partial k}{\partial z} + \rho u \frac{\partial k}{\partial r} - \frac{1}{r} \left[\frac{\partial}{\partial z} \left(r \mu_k \frac{\partial k}{\partial z} \right) + \frac{\partial}{\partial r} \left(r \mu_k \frac{\partial k}{\partial r} \right) \right] = G - \rho \epsilon \quad (16)$$

$$\rho w \frac{\partial \epsilon}{\partial z} + \rho u \frac{\partial \epsilon}{\partial r} - \frac{1}{r} \left[\frac{\partial}{\partial z} \left(r \mu_\epsilon \frac{\partial \epsilon}{\partial z} \right) + \frac{\partial}{\partial r} \left(r \mu_\epsilon \frac{\partial \epsilon}{\partial r} \right) \right] = \frac{C_1 G \epsilon}{k} - \frac{C_2 \rho \epsilon^2}{k} \quad (17)$$

$$\frac{G}{\mu_t} = 2 \left(\left(\frac{\partial w}{\partial z} \right)^2 + \left(\frac{\partial u}{\partial r} \right)^2 + \left(\frac{u}{r} \right)^2 \right) + \left(\frac{\partial w}{\partial r} + \frac{\partial u}{\partial z} \right)^2 \quad (18)$$

where, $\mu_k = \mu + \mu_t / \lambda_k$, $\mu_\epsilon = \mu + \mu_t / \lambda_\epsilon$, $\lambda_k = 1$, $\lambda_\epsilon = 1.3$, $C_1 = 1.44$, $C_2 = 1.92$, $C_3 = .09$. These equations are solved along with the Navier-Stokes equations (Eq. 13) using,

$$\begin{aligned} \phi &= k, a_\phi = 1, b_\phi = r \mu_k, c_\phi = 1, d_\phi = r(G - \rho \epsilon) \\ \phi &= \epsilon, a_\phi = 1, b_\phi = r \mu_\epsilon, c_\phi = 1, d_\phi = r(C_1 G \epsilon / k - C_2 \rho \epsilon^2 / k) \end{aligned}$$

2.3 Boundary and Initial Conditions. The boundaries of the inner grenade chamber (see Figure 1) are the inlet (connected to the pyrotechnic chamber), the exit (nozzle throat), the symmetry axis, the chamber wall lined with payload material, and a section of solid wall along the nozzle. Since the governing equations (Eq. 13) are elliptic the conditions along these boundaries must prescribe values of the dependent variables, the gradient of the dependent variables in the normal direction, or an algebraic relation which connects the values of the dependent variables to the normal component of velocity.

At the inlet plane, radial profiles of all dependent variables, $\psi, \omega, m_j, \tilde{h}, v, k$, and ϵ as well as values for V, T, p, ρ , and μ_{eff} are specified. It is assumed that the flow at the inlet plane consists of air and that the diffusion of payload into the airstream from the chamber wall does not effect the inlet flow. During actual grenade operation the inlet flow consists of pyrotechnic combustion gases (e.g. $\text{H}_2\text{O}, \text{CO}_2$) the exact nature of which was unavailable for the numerical simulations. A subsonic inlet flow velocity assumption is used in accordance with the elliptic nature of the governing equations. Initial conditions for all dependent variables are supplied by the inlet boundary conditions. The turbulence model is initialized using $k = k_\infty = \alpha V_\infty^2$, $\epsilon = k^{1.5} C_3^{-0.5} / (.37 x^{0.8} \text{Re}^{-0.4})$. The initial turbulence kinetic energy is specified as $(1/\alpha)\%$ of the inlet kinetic energy.

The exit plane is located at the nozzle throat where the flow is assumed to be subsonic. The streamlines at the exit plane are assumed to be parallel to the symmetry axis; thus, the gradients of all dependent variables along these streamlines are zero. These assumptions are

reasonable since experience for large Reynolds numbers has shown that the exact nature of the exit plane boundary conditions has little effect on the flowfield solution when convection is significant (i.e. large inlet mass flow) (Bradshaw et.al. 1981, Khalil et.al. 1975).

For mass continuity, the symmetry axis is considered to be a streamline of the flow, thus $\psi = \text{constant}$. Along the symmetry axis $r = 0$, thus $\partial\psi/\partial z = \partial\psi/\partial r = 0$ via Equation 12. The value of ψ along this boundary can be determined from values of ψ adjacent to the boundary using a one-sided finite-difference for $\partial\psi/\partial r$ at the axis. From Equation 12, the boundary value for ω is zero. The axis boundary values for the remaining dependent variables, ϕ , are determined from $\partial\phi/\partial r = 0$.

The no-slip condition ($u = w = 0$, and $v/r = \Omega$, where Ω is the wall spinrate) is applied to the solid walls. Therefore $\psi = \text{constant}$, via Equation 12. For convenience $\psi = 0$ is chosen. One-sided finite-differences for $\partial\psi/\partial r$ and $\partial\psi/\partial z$ are used in Equation 12 to determine the wall value for ω . For an inert wall, the normal gradient of all mass fractions, $\partial m_j/\partial n$, are set to zero. For a wall with payload material, the boundary condition is based on the assumption that the payload material is continually vaporizing ($m_{\text{payload}} = 1, m_{\text{air}} = 0, m_{\text{mixture}} = 0$). The wall temperature is set to the vaporization temperature of the payload, $T_{\text{wall}} = T_{\text{vap}}$. Figure 2 shows the results of a thermogravimetric analysis of yellow dye (i.e. payload material) (Turetsky 1991). The percent weight loss of the sample is plotted as a function of temperature. Note that vaporization of the material (i.e. significant weight loss) occurs over a narrow temperature range, supporting the use of such a boundary condition. The rate of burning (regression rate) on the payload surface varies as a function of position along the surface and is computed from the temperature gradient normal to the wall,

$$\dot{r} = \frac{-\kappa_p}{\rho_p h_{\text{vap}}} \frac{\partial T}{\partial r} \quad (19)$$

where κ_p and ρ_p are the thermal conductivity and density of the solid payload, and h_{vap} is the heat of vaporization of a unit mass of payload. Values of the thermal conductivity, density, and heat of vaporization can be determined for most grenade payload materials.

The boundary conditions for the payload surface are based on the assumption of single diffusion, i.e. diffusion of gaseous payload molecules into the airstream without diffusion of air molecules into the payload material. Single diffusion has been studied by R.D. Present (1958). The general equation of mutual/thermal diffusion is given by,

$$G_j = n_j u_j - n \Gamma \frac{d}{dz} \left(\frac{n_j}{n} \right) + \frac{n_j \Gamma_T}{T} \frac{dT}{dz} \quad (j = 1, 2) \quad (20)$$

where n_j = molecular density of species j , $n = \sum_j n_j$, u_j = convection velocity of species j , z = diffusion direction, Γ = mass diffusion coefficient ($V\lambda/3$, λ = the molecular mean free path), and Γ_T = thermal diffusion coefficient ($\kappa/(\rho h_{\text{vap}})$). The equation of "single diffusion"

can be obtained by assuming that air molecules ($j=1$) are moving in a boundary layer so that $u_1 \simeq 0$ and payload molecules ($j=2$) are at rest, $u_2 \equiv 0$. In addition, the payload molecules are closely packed so that $n_1 \ll n_2$. As a result,

$$G_{\text{air}} = G_1 \simeq 0, \quad G_{\text{payload}} = G_2 \simeq -(n_1 + n_2)\Gamma \frac{d}{dz} \left(\frac{n_2}{n_1 + n_2} \right) + \frac{n_2\Gamma_T}{T} \frac{dT}{dz} \quad (21)$$

The mass diffusion terms of Equation 21 are incorporated in the J_j terms of Equation 5 and Γ_T is customarily neglected.

The payload surface boundary condition may also be prescribed using a surface ablation model such as described by Moss (1976). In this model the payload vaporization temperature and heat of vaporization are prescribed as functions of the pressure applied to the material surface. An equation similar to Equation 19 is used along with these functions in a iterative/coupling procedure with the governing equations in order to prescribe the payload surface boundary condition. The use of an ablation model, as opposed to assuming that the payload surface is continually vaporizing ($T_{\text{wall}} = T_{\text{vap}}$) is more critical for cases where the vaporization characteristics of the material are a strong function of pressure and temperature (i.e. unlike that shown in Fig. 2). The major drawback to using an ablation model is the increased computational cost of the iterative procedure and the requirement of experimental data in the form $T_{\text{vap}} = T_{\text{vap}}(p)$, $h_{\text{vap}} = h_{\text{vap}}(p)$.

Boundary conditions for turbulence variables, k and ϵ , are $k = 0$, $\epsilon = .056\mu(\partial u/\partial r)^2/\rho$ for solid walls and $k = 10^{-6}V_\infty^2$, $\epsilon = k^{1.5}/L$ for the inlet flow. Along the chamber axis and exit plane $\partial k/\partial r = \partial \epsilon/\partial r = 0$, $\partial k/\partial z = \partial \epsilon/\partial z = 0$, respectively.

2.4 Computational Algorithm. Equation 13 can be reduced to a successive-substitution formula for flow variable ϕ at each node on the computational grid. Central finite-differences are used for the diffusive and source terms and upwind differences for the convective terms. Using upwind differencing in the species conservation equations (Eq. 5) reduces the occurrence of negative species mass fractions in mixing layers. The resulting system of equations for the entire grid is solved using a Gauss-Seidel relaxation scheme (Nusca 1989). Each iteration cycle is made up of M sub-cycles, where M is the number of equations being considered (M must be at least 2 since the equations for $\phi = \omega/r$ and $\phi = \psi$ are the minimum required to define the flow). In each sub-cycle, grid points are scanned row by row and a single variable is updated. The variables ω/r and ψ are updated in order followed by all other variables. When all sub-cycles are completed a new iteration cycle is started in which the values of the variables from the latest iteration are immediately used. This is consistent with the Gauss-Seidel methodology (Carnahan 1969). Convergence is satisfied when the greatest relative change in any flow variable is smaller than a prescribed tolerance.

3. RESULTS

In order to demonstrate the numerical method, simulations were performed for an experimental grenade model loaded with yellow dye payload simulant that has been the subject of testing at CRDEC. In these tests the grenade's inner chamber was instrumented with pressure transducers and thermocouples (for temperature measurements). The chamber was lined with yellow dye payload material about .25 inches in thickness. A typical test run yields measured values for the chamber inlet pressure and temperature (due mainly to pyrotechnic ignition) of about 3.5 psig (1.24 atm) and 425 C. The nozzle or exit plane values were measured as 1.5 psig (1.1 atm) and 375 C. These values were used as boundary conditions for the numerical simulation. The chemical properties of the yellow dye payload material were measured as $T_{\text{vap}} = 241$ C, $h_{\text{vap}} = 102.9$ J/g, $\mathcal{M} = 273$ g/mole. The density and thermal conductivity of the dye have not been measured but were taken as $\rho_p = 1.8$ g/mole and $\kappa_p = .00143$ cal/s-cm-C, respectively. Sensitivity studies using the present numerical model show that the predicted payload regression rate depends significantly on the value of κ_p and less on the value of ρ_p . The inlet gas was assumed to be air with $\mathcal{M} = 28.8$ g/mole and the \mathcal{M} of the air/payload gas mixture taken as 150 g/mole.

Figure 3 shows the computational grid (or mesh) used for flowfield simulation within the grenade's inner chamber, bounded axially by the inlet and nozzle and radially by the symmetry axis and chamber wall. The chamber is cylindrical with an overall length of 4.0 inches and .375 inches in diameter. These dimensions represent the chamber shape before payload surface regression. Note that the vertical axis in Figure 3 has been magnified for clarity by a factor of 10 over the horizontal axis. About 131 grid points were used in the axial direction with 35 points in the radial direction; the grid points were unevenly distributed in order to cluster points along the boundaries (except at the symmetry axis). Figure 4 shows the computed velocity vectors (i.e. arrows whose length is representative of the magnitude of local gas velocity and direction indicates the orientation of the local velocity) displayed at every 6th axial grid point and every other radial point (for clarity). A thick boundary layer that develops along the chamber wall (i.e. payload surface) can be observed. The computed average chamber exit velocity is approximately 121 ft/s. The surface of the payload material was allowed to ablate (i.e. regress) for .25 seconds resulting in the shape shown in Figure 5 (computational grid). Note that the material surface has been blunted at the chamber inlet but more evenly eroded over most of the surface with the exception of a discontinuity at the payload/nozzle wall junction ($z = 3.5$ inches). Figure 6 shows the computed velocity vectors for this chamber shape. Due to the contour of the chamber entrance, the flow is significantly accelerated (indicated by longer arrows in the figure) forming a thinner boundary layer along the payload surface (i.e. larger Re). The computed average chamber exit velocity is

approximately 276 ft/s. Figure 7 shows the distribution of payload regression rate (Eq. 19) along the payload surface for both the initial time and .25 seconds elapsed time. Payload regression rate is largest near the chamber inlet and nearly uniform over most of the payload surface. The regression rate increases with elapsed time.

Figure 8 shows radial profiles of axial velocity component at both the initial and elapsed time as well as two axial positions along the chamber - midlength, $z = 2\text{in}$, and the exit plane, $z = 4\text{in}$. Consistent with the imposed boundary conditions the velocity is zero at the chamber wall ($r = .1875\text{in}$) and the velocity gradient is zero at the chamber axis ($r = 0$). The retarding effect of the wall boundary layer on the velocity profile can also be observed. Note that the profiles at chamber midlength show the payload surface regressing from $r = .1875\text{in}$ to about $.195\text{in}$ from the centerline while the profiles at chamber exit show no wall regression since the chamber wall is solid at this location. Comparing the chamber midlength profiles with those at the exit plane show that the boundary layer (or mixing layer) thickens with axial location downstream of the inlet. Comparing the initial time profiles with those at the elapsed time show that the gas flow is significantly accelerated as the payload surface regresses and the boundary layer thickness decreases (i.e. larger Re).

Figure 9 shows radial profiles of gas temperature at both the initial and elapsed time as well as two axial positions along the chamber - midlength, $z = 2\text{in}$, and the exit plane, $z = 4\text{in}$. Consistent with the imposed boundary conditions the temperature is T_{vap} at the payload surface while the temperature gradient is zero at both the chamber axis and the solid chamber wall at the nozzle (adiabatic wall condition). Note that the profiles at chamber midlength show the payload surface regressing from $r = .1875\text{in}$ to about $.195\text{in}$ from the centerline while the profiles at chamber exit show no wall regression since the chamber wall is solid at this location. Within the boundary layer established on the payload surface the temperature of the air/payload mixture is gradually increased until it reaches the centerline (i.e. inlet) value. Comparing the chamber midlength profiles with those at the exit plane show that the thermal boundary layer thickens with axial location downstream of the inlet. Comparing the initial time profiles with those at the elapsed time show that the gas flow is slightly hotter at any chosen radial position within the mixing layer.

Figures 10 and 11 show radial profiles of mixture (payload + air) mass fraction at both the initial and elapsed time as well as two axial positions along the chamber - midlength, $z = 2\text{in}$, and the exit plane, $z = 4\text{in}$. Consistent with the imposed boundary conditions the mixture mass fraction, m_{mixture} , is zero at the payload surface (i.e. $m_{\text{payload}} = 1$, $m_{\text{air}} = 0$) and along the chamber centerline (i.e. $m_{\text{payload}} = 0$, $m_{\text{air}} = 1$). Along solid walls (i.e. chamber exit) and at the chamber centerline the gradient of m_{mixture} is zero. The mixture mass fraction is exactly or nearly unity at some point in the flowfield where m_{payload} and

m_{air} are equivalent. Note that the profiles at chamber midlength show the payload surface regressing from $r = .1875\text{in}$ to about $.195\text{in}$ from the centerline while the profiles at chamber exit show no wall regression since the chamber wall is solid at this location. Comparing the chamber midlength profiles with those at the exit plane show that the chamber core flow, consisting of air ($m_{\text{mixture}} = 0$), thins from a radial position of about $.12\text{in}$ to $.10\text{in}$ at the initial time and $.15\text{in}$ to $.13\text{in}$ at the elapsed time. The diffusion of payload material into the core flow is advanced with axial position as the boundary layer imposed on the payload surface grows. Comparing the initial time profiles with those at the elapsed time show that the mixing layer (i.e. highest mixture concentration) follows the payload surface as regression progresses.

4. CONCLUSIONS

Material dissemination from the payload chamber inside a dual-chamber grenade has been simulated using computational fluid dynamics. A thermal dissemination technique that uses the hot, moving gases generated from combustion of a pyrotechnic within the grenade has been investigated. The dissemination process is initiated by ablation and vaporization of the payload material from exposure to the thermal effects of pyrotechnic combustion. This material in gaseous form is entrained in this flow and expelled from the grenade. The Navier-Stokes equations along with chemical species conservation equations were used to simulate the diffusion and convection processes of the flowfield within the grenade's payload chamber. Numerical simulations reveal that diffusion of the payload material is accomplished within a boundary layer that is established along the payload surface (chamber wall) and that a core flow, basically unaffected by the payload ablation, resides over about one-half of the chamber diameter. Thermal exposure of the payload mixture to the hot combustion gases from the pyrotechnic is concentrated in this layer where the temperature is below that of the core flow gases. As the payload surface regresses, the flow thru the chamber is accelerated and the diffusion/mixing layer follows the regressing surface which results in an expansion of the core flow. The regression rate increases with elapsed time (since pyrotechnic ignition) as the shape of the payload surface (chamber wall) is contoured by material ablation.

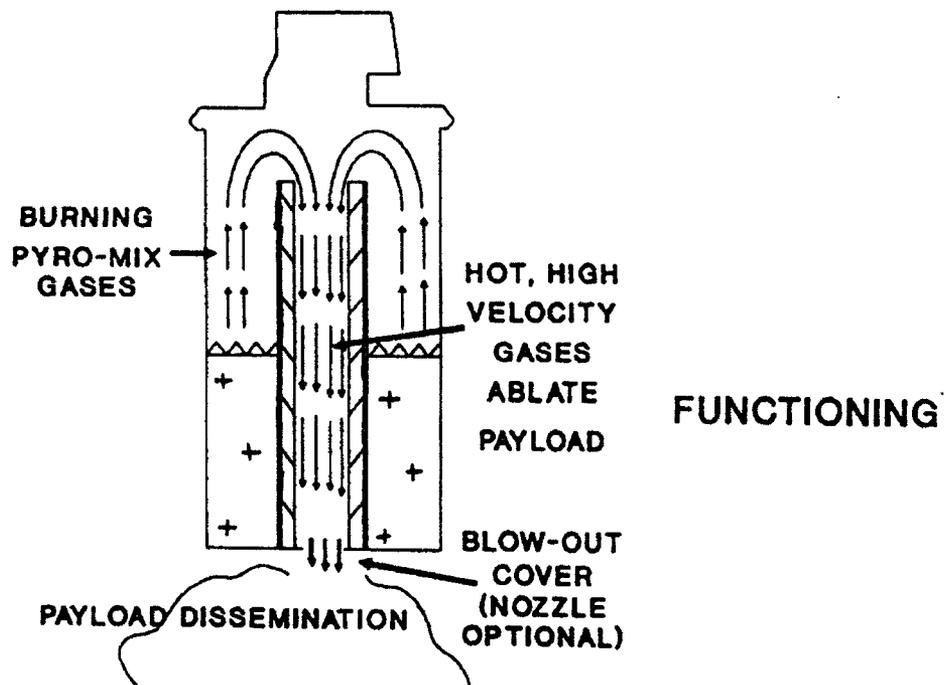
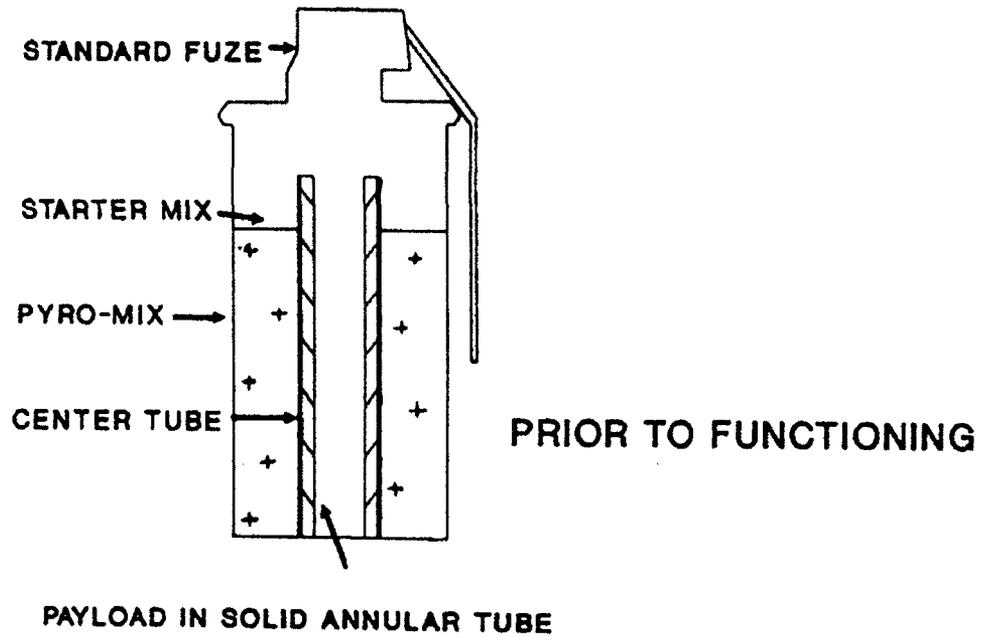


Figure 1. Schematic showing operation of the dual-chamber grenade thermal dissemination (M. Miller, U.S. Army CRDEC, used with permission)

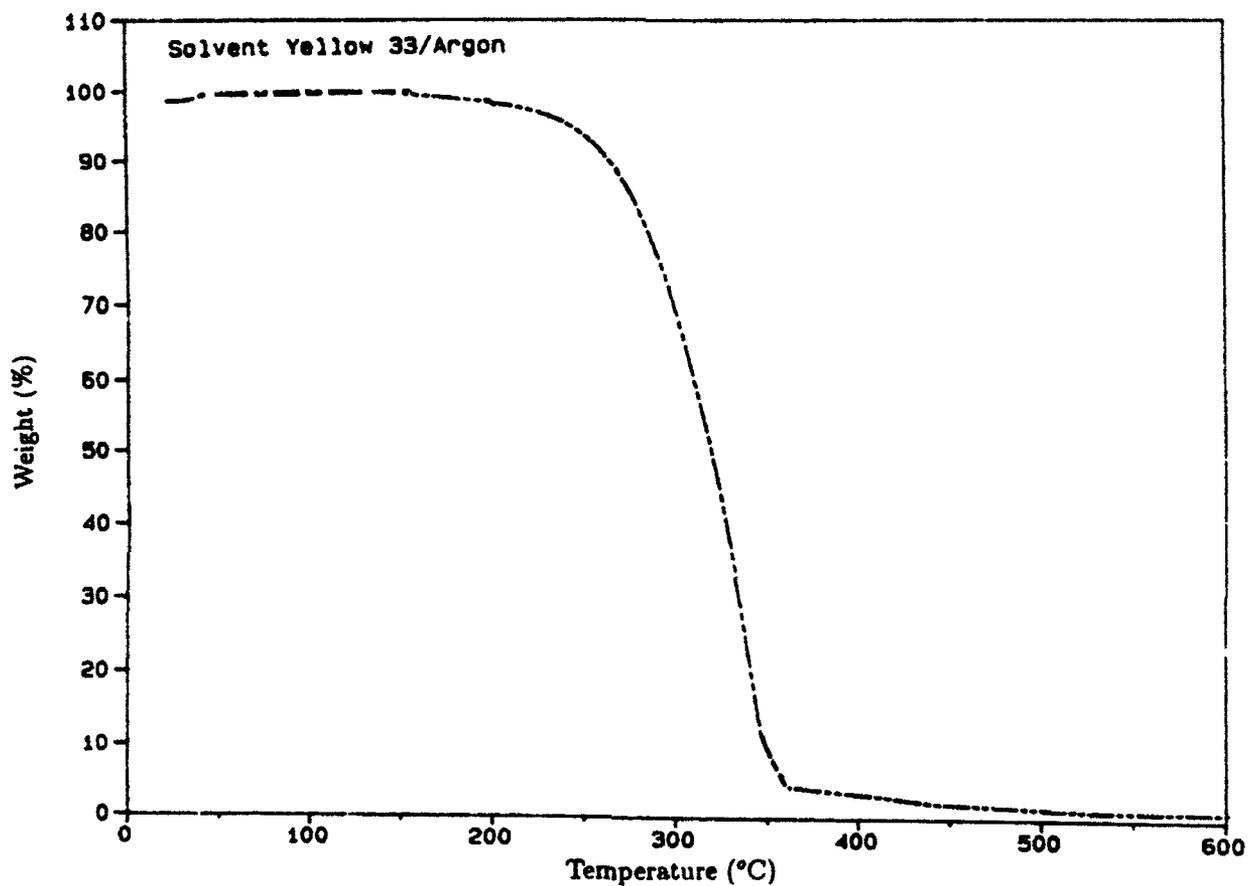


Figure 2. Measured weight change (%) of solvent yellow dye sample during heating from 0 to 600 C in argon atmosphere. Measurements done using thermogravimetric analyzer at CRDEC (Turetsky 1991)

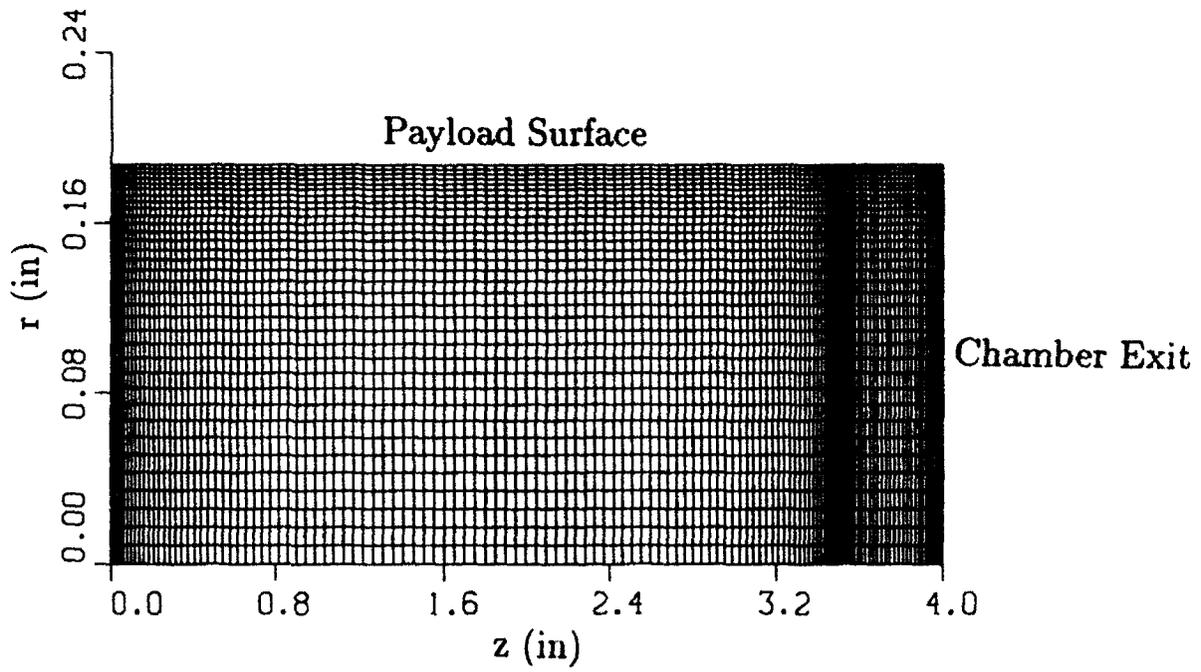


Figure 3. Computational grid for initial chamber shape

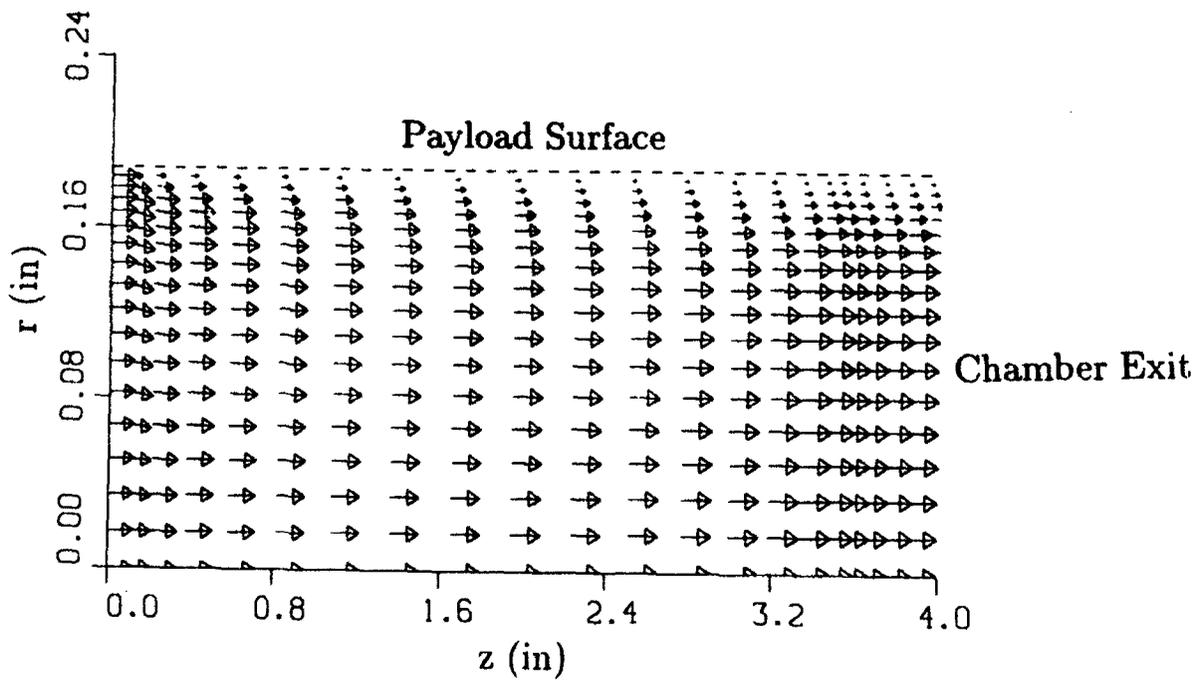


Figure 4. Computed velocity vector field for initial chamber shape

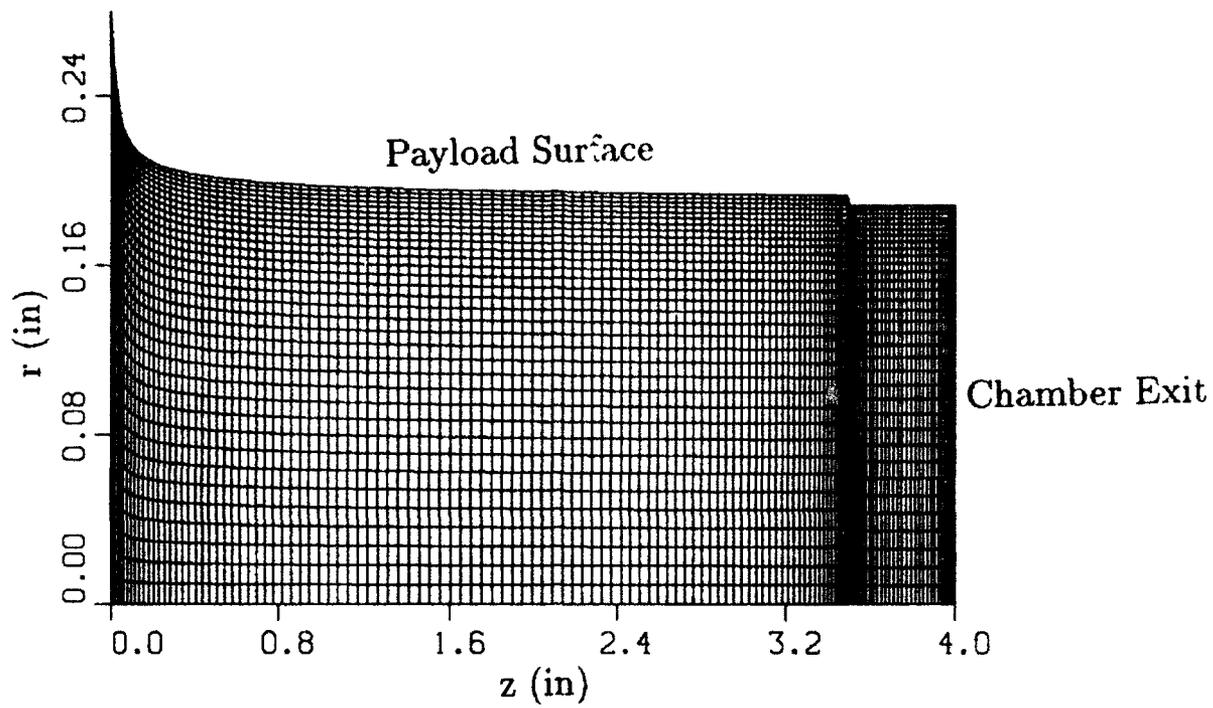


Figure 5. Computational grid for chamber shape after .25 seconds of payload surface ablation

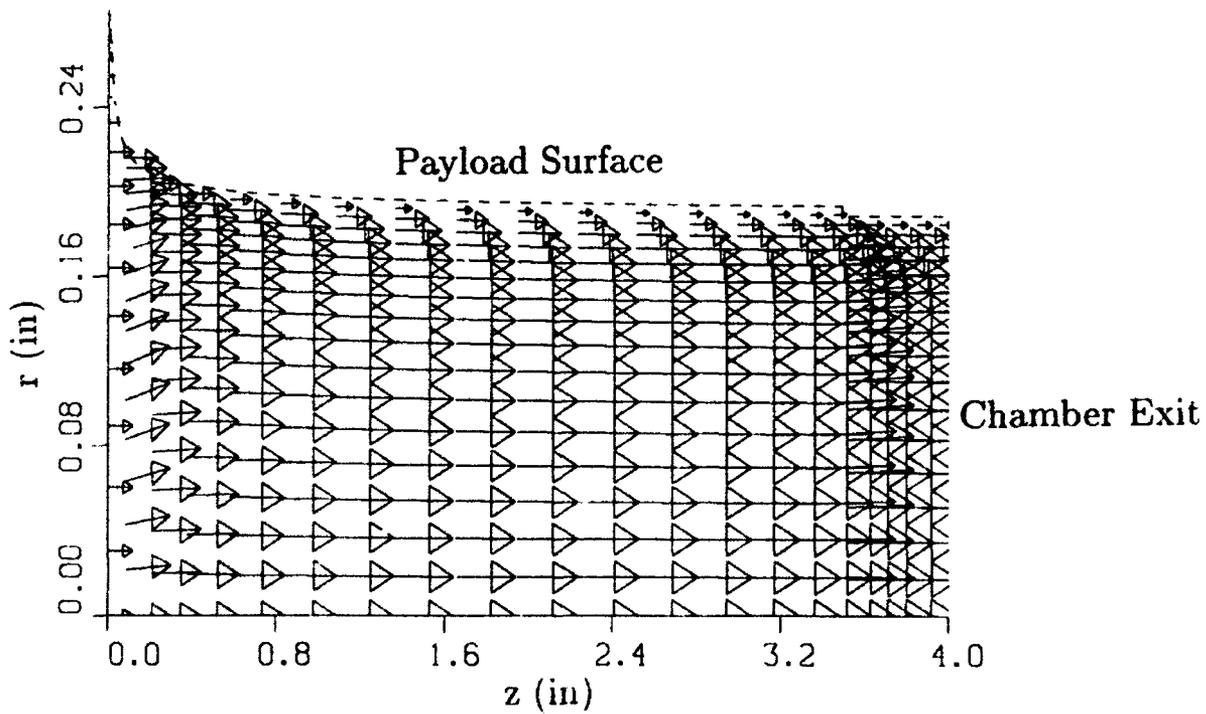


Figure 6. Computed velocity vector field for chamber shape after .25 seconds of payload surface ablation

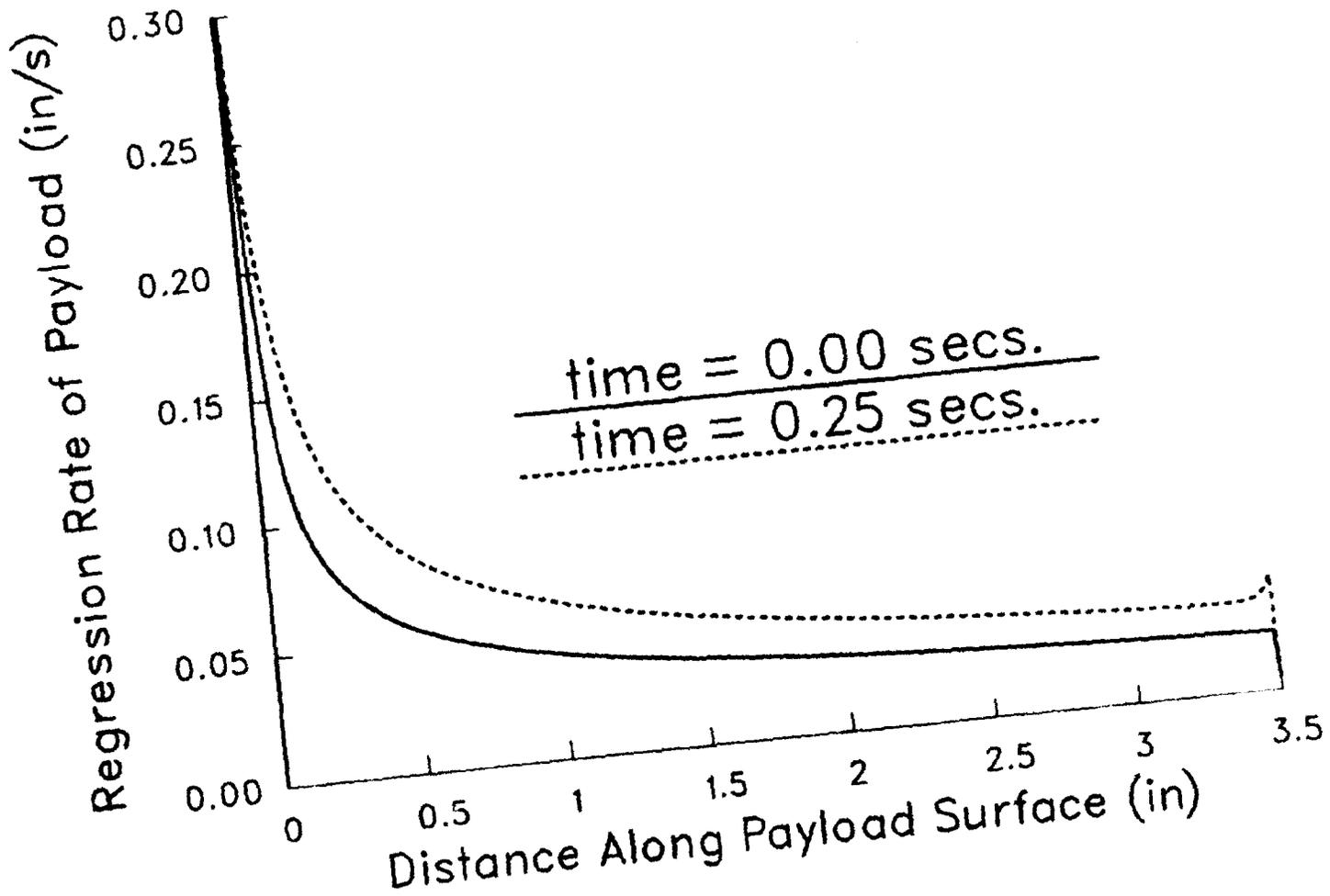


Figure 7. Computed payload material regression rate as a function of distance along payload surface, results for initial and elapsed time shown

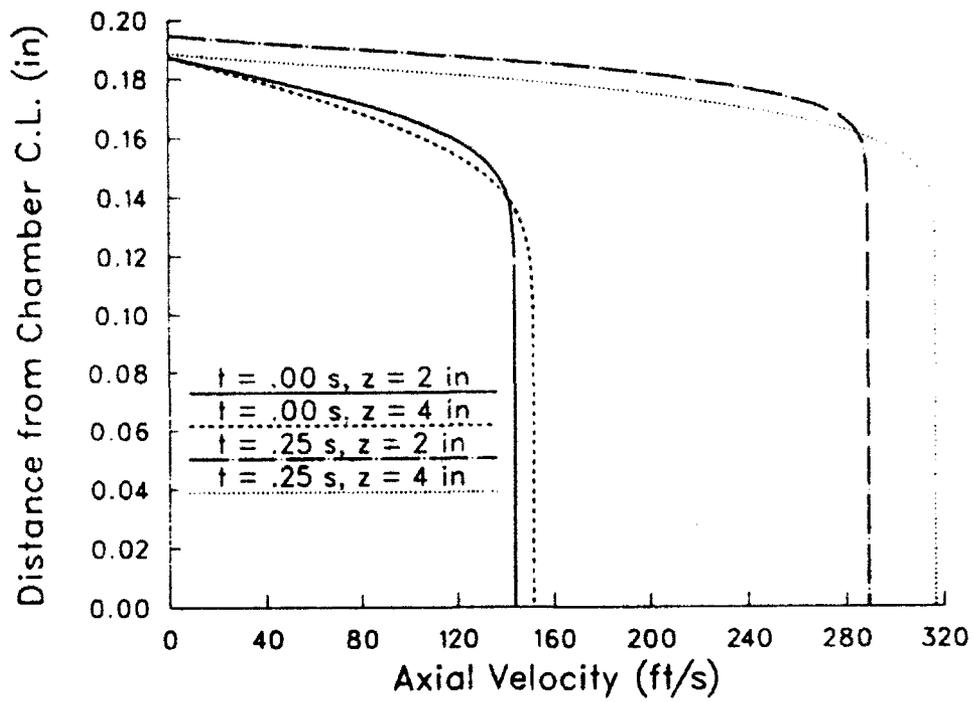


Figure 8. Computed radial profiles of axial component of gas flow velocity; results for initial and elapsed time shown at the chamber midlength and nozzle exit

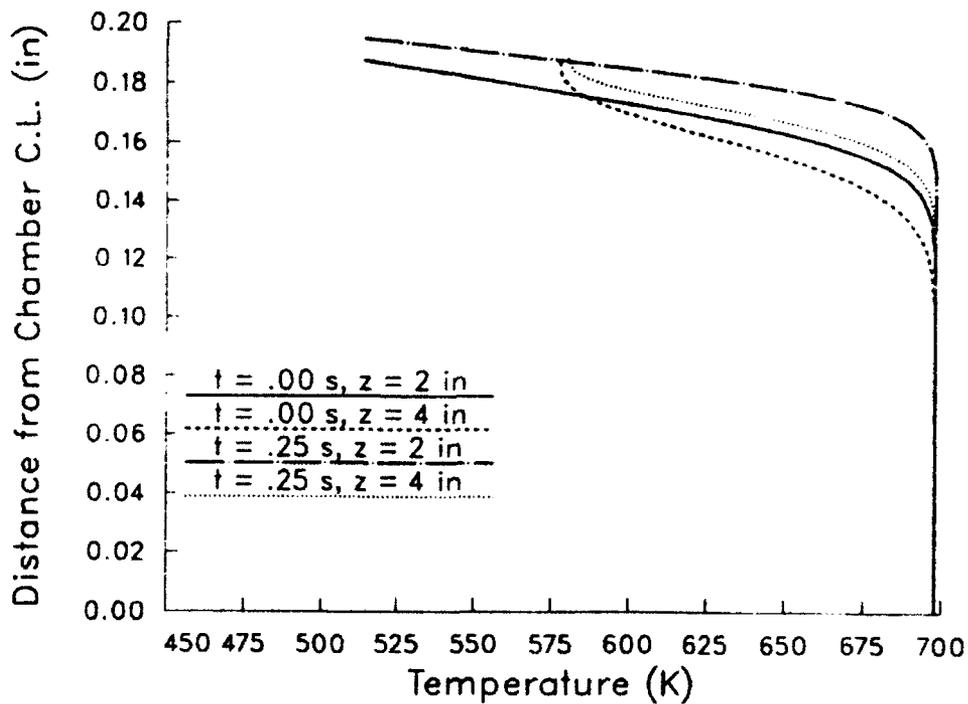


Figure 9. Computed radial profiles of gas temperature; results for initial and elapsed time shown at the chamber midlength and nozzle exit

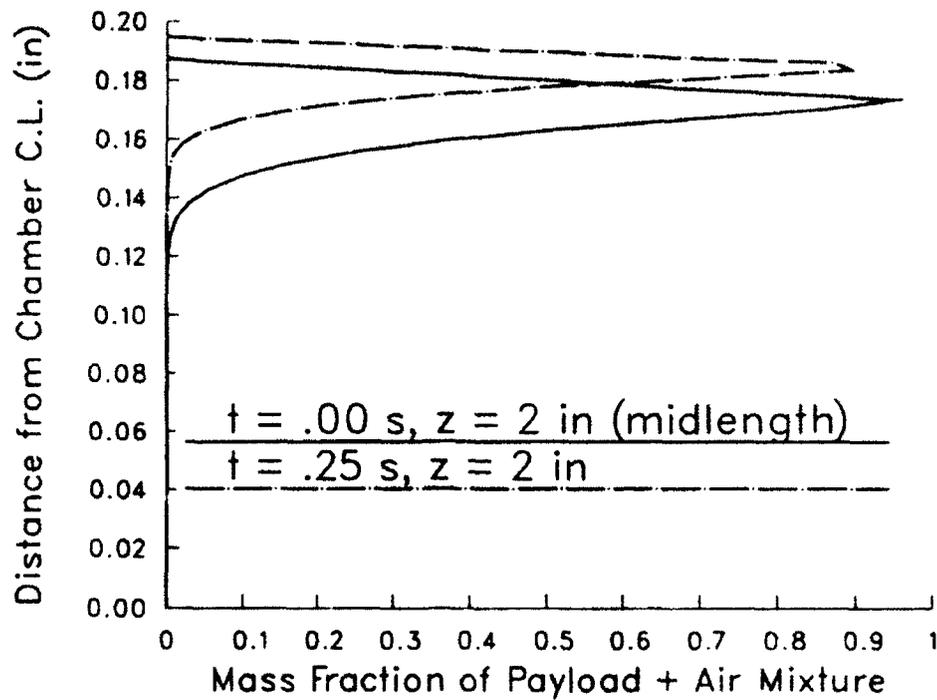


Figure 10. Computed radial profiles of gas composition (mixture mass fraction); results for initial and elapsed time shown at the chamber midlength

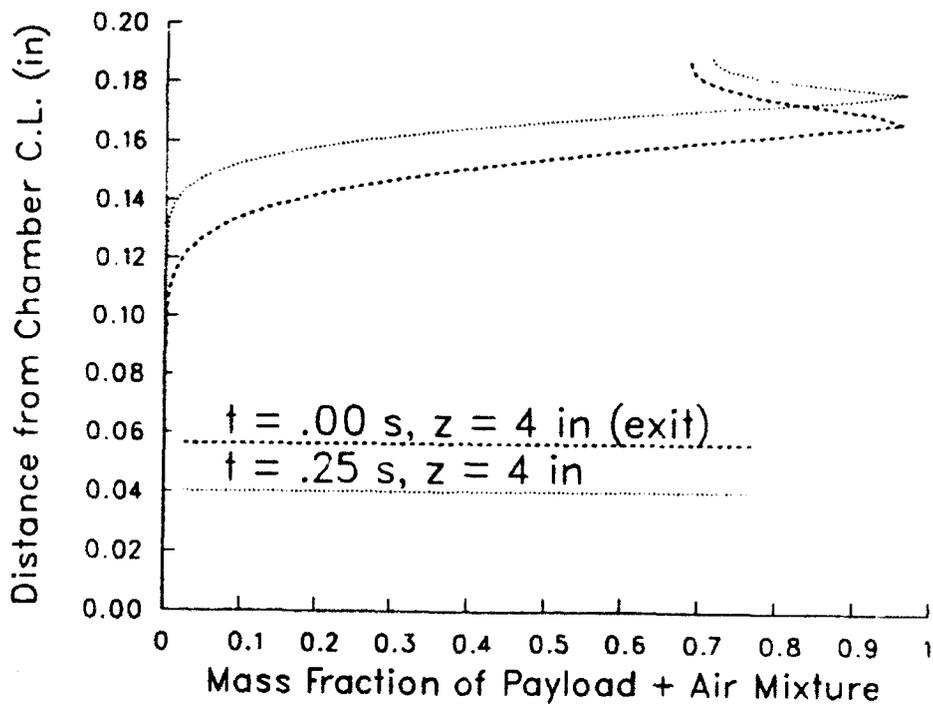


Figure 11. Computed radial profiles of gas composition (mixture mass fraction); results for initial and elapsed time shown at the chamber nozzle exit

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LIST OF SYMBOLS

c_p	specific heat capacity, constant p
h	molar specific enthalpy
\tilde{h}	total enthalpy
h_{vap}	payload material heat of vaporization
J	flow rate or flux
k	turbulence kinetic energy
L	characteristic length
m	species mass fraction
\mathcal{M}	molecular weight
n	molecular density
N	number of species
p	static pressure
Pr	Prandtl Number
r	radial direction
\dot{r}	payload surface regression rate
\mathfrak{R}	specific gas constant, $(\gamma - 1)c_p/\gamma$
$\bar{\mathfrak{R}}$	universal gas constant, $\mathfrak{R} \sum_j \mathcal{M}_j$
Re	Reynolds Number
Sc	Schmidt Number
t	time
T	static temperature
u	radial velocity component
v	azimuthal velocity component
V	magnitude of the local velocity vector
\vec{V}	$u\hat{r} + v\hat{\theta} + w\hat{z}$
w	axial velocity component
X	mole fraction
z	axial direction

Greek Symbols

γ	ratio of specific heats
Γ	diffusion coefficient
ϵ	turbulence dissipation rate
θ	azimuthal direction
κ	thermal conductivity
μ	molecular viscosity
ρ	density
$\vec{\tau}$	shear stress vector
ϕ	general flow variable
ψ	stream function
ω	vorticity

Superscripts

$\hat{\cdot}$	unit vector
$\bar{\cdot}$	total or stagnation quantity
$\dot{\cdot}$	rate

Subscripts

eff	effective
h	enthalpy contribution
j	j -th mixture component or species
k	turbulence kinetic energy contribution
p	constant pressure
p	payload quantity
r	radial component or radial direction
t	turbulence quantity

z axial component
 ϵ turbulence dissipation rate
 θ azimuthal component
 ∞ freestream quantity

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