THERMOBARIC EXPLOSIVES

TBX (a thermobaric explosive) is defined as "a *partially detonating energetic material with excess fuel (gas, solid or liquid) dispersed and mixed into air with subsequent ignition and reaction achieved in time and in place for added gain of energy, blast and heat.*" That is, TBX has greatly enhanced thermal and blast effects compared to conventional high explosives [1]. In general, it contains metal particles such as aluminum and magnesium in oxygen-deficient composition. In TBX flow, thermobaric effects are obtained by long-duration overpressure and heating due to the afterburning of detonation products in air. Since the afterburning process is controlled by turbulent mixing and combustion in air after detonation or dispersion by a bursting charge, even the identical explosive composition may yield different thermal and blast performance with different targets. Therefore, the detailed understanding of the afterburning mechanism is required to optimally design warheads for various operational environments.

TNT explosions in air have been investigated for a long time due to the importance of explosive physical phenomenon widely used in the military and security industries. In general, TNT explosions that propagate into a confined area generally undergo two consecutive stages: initial blast (or the first fireball) and afterburning (or the second fireball). During the first fireball process, which is extremely oxygen deficient, the solid explosive of the TNT transforms into the gaseous detonation products mainly consisting of carbon dust, C(s) and carbon monoxide, CO in a fairly small confined region. In the second process which typically is an explosion in air with excess oxygen, the generated carbon dust and carbon monoxide can serve as a fuel that burns with a certain amount of oxygen in such a manner that the solid carbon is converted to carbon monoxide followed by conversion of carbon monoxide to carbon dioxide, CO₂. It is experimentally proven that the secondary fireball is much more energetic than the first fireball for TNT blast, and encompasses a fairly large region compared to the initial blast [2, 3]. In addition, since the afterburning process encompasses the blast propagation, shock reflections, and turbulent mixing in an extremely high pressure and temperature environment inherited from the initial TNT blast, it is extremely difficult to understand the complex physics involved.

THEORETICAL MODEL

In the first fireball region near the initial explosive charge, solid TNT which is extremely oxygen deficient transforms into the following detonation products: C(s), CO, $H_2O(g)$, and N_2 . After this process, a second explosion involving excess oxygen follows, using the carbon dust and carbon monoxide as a substitute fuel reacting one after the other. Since the volume containing and immediately surrounding the TNT charge is very small compared to the total enclosure confined, our approach for the thermobaric blast modeling in this report is mainly focused on the secondary fireball region. The theoretical model in this region has two features: a detonating gas phase and a dispersed aluminum particle phase. In the gas phase, we derive conservation equations which are appropriate for supersonic multiphase chemically reactive flows. In addition, comprehensive source terms which are the main key for the multiphase flow with a dispersed particle phase are also described in detail. In the dispersed phase, we applied an empirical quasi-steady burning law instead of the conventional diffusion-based evaporation model, and all dispersed equations based on the mass, momentum, and energy conservation equations governing the particle properties are comprehensively derived in an Eulerian coordinate system. In both phases, the combustion models are developed based on infinitely fast reactions, in which all species involving exploding gas and aluminum particle combustion are considered.

1 GAS PHASE MODEL

The conservation equations governing the unsteady, explosive detonating gas with exothermic and aluminum particle combustion can be expressed as 2-dimensional Euler equations in axisymmetric coordinates, or 3-dimensional Euler equations in a rectangular coordinate system.

2-DIMENSIONAL FORM

The combined vector form of the governing equations in 2-dimensional coordinates is summarized as:

$$\frac{\partial \vec{u}}{\partial t} + \frac{\partial E\left(\vec{u}\right)}{\partial x} + \frac{\partial F\left(\vec{u}\right)}{\partial y} = G\left(\vec{u}\right) + S\left(\vec{u}\right) + W\left(\vec{u}\right)$$
(1.1)

where x, $y \ge 0$, and t are the axial and radial coordinates, and time, respectively. The primitive flow variable \vec{u} , and the flux vectors, $E(\vec{u})$ and $F(\vec{u})$, are described as:

$$\vec{u} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho E \\ \rho_1 \\ \rho_2 \\ \rho_3 \\ \vdots \\ \rho_{n-1} \end{bmatrix} , E(\vec{u}) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \\ \rho_1 u \\ \rho_2 u \\ \rho_3 u \\ \vdots \\ \rho_{n-1} u \end{bmatrix} , F(\vec{u}) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \\ \rho_1 v \\ \rho_2 v \\ \rho_3 v \\ \vdots \\ \rho_{n-1} v \end{bmatrix}$$
(1.2)

Here, ρ , u, v, p, and E are density, velocities, pressure, and specific total energy of the gas mixture, and ρ_i for i = 1, ..., n-1 are the mass density of species i, which are involved in exothermic and aluminum particle combustion. The source terms $G(\vec{u})$, $S(\vec{u})$, and $W(\vec{u})$ in the axisymmetric geometry case represent the coupling exchange between the explosive gas and solid aluminum particle, and the chemical reactions are described as:

where s_i , s_{ii} , s_{ii} , s_{ii} , s_{ii} , and s_i are the exchange terms representing mass, momenta, energy, and generation of the aluminum vapor by evaporation. The source terms $\dot{\omega}_i$ for $i = 1, 2, \dots, n-1$ in the species equation are the production rates of species *i* by the chemical reactions involved.

3-DIMENSIONAL FORM

The combined vector form of the governing equations in 3-dimensional coordinates is also summarized as:

$$\frac{\partial \vec{u}}{\partial t} + \frac{\partial E\left(\vec{u}\right)}{\partial x} + \frac{\partial F\left(\vec{u}\right)}{\partial y} + \frac{\partial G\left(\vec{u}\right)}{\partial z} = S\left(\vec{u}\right) + W\left(\vec{u}\right)$$
(1.4)

where x, y, z, and t are the rectangular spatial coordinates, and time, respectively. The primitive flow variables \vec{u} , and the flux vectors, $E(\vec{u})$, $F(\vec{u})$ and $G(\vec{u})$, are described as:

$$\vec{u} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho v \\ \rho w \\ \rho w \\ \rho E \\ \rho_{1} \\ \rho_{2} \\ \rho_{3} \\ \vdots \\ \rho_{N-1} \end{bmatrix}, E(\vec{u}) = \begin{bmatrix} \rho u \\ \rho u^{2} + p \\ \rho uv \\ \rho uw \\ \rho vw \\ \nu(\rho E + p) \\ u\rho_{1} \\ u\rho_{2} \\ u\rho_{3} \\ \vdots \\ u\rho_{N-1} \end{bmatrix}, F(\vec{u}) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho vv \\ \rho v^{2} + p \\ \nu(\rho E + p) \\ v\rho_{1} \\ v\rho_{2} \\ v\rho_{3} \\ \vdots \\ v\rho_{N-1} \end{bmatrix}, \text{ and } G(\vec{u}) = \begin{bmatrix} \rho w \\ \rho uw \\ \rho w \\ \rho w \\ \rho w \\ \rho w \\ \rho w^{2} + p \\ w(\rho E + p) \\ w\rho_{1} \\ w\rho_{2} \\ w\rho_{3} \\ \vdots \\ w\rho_{N-1} \end{bmatrix} (1.5)$$

Here, ρ , u, v, p, and E are density, velocities, pressure, and specific total energy of the gas mixture, and ρ_i for i = 1, ..., n-1 are the mass densities of species i that is involved in exothermic and aluminum particle combustion. The source terms $S(\vec{u})$ and

 $W(\vec{u})$ representing a coupling exchange between the explosive gas and solid aluminum particle, and the chemical reactions are also described as:

$$S(\vec{u}) = \begin{bmatrix} s_{I} \\ s_{III} \\ s_{III} \\ s_{IV} \\ s_{V} \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ s_{i} \\ \vdots \\ 0 \end{bmatrix}, \text{ and } W(\vec{u}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \dot{w}_{1} \\ \dot{w}_{2} \\ \dot{w}_{3} \\ \vdots \\ \dot{w}_{i} \\ \vdots \\ \dot{w}_{i} \\ \vdots \\ \dot{w}_{n-1} \end{bmatrix}$$
(1.6)

where s_I , s_{II} , s_{III} , s_{IV} , s_V , and s_i are the exchange terms representing mass, momenta, energy, and generation of the aluminum vapor by evaporation. The source terms $\dot{\omega}_i$ for $i = 1, 2, \dots, n-1$ in the species equation are the production rate of species *i* of chemical reactions involved. In addition, since

$$\rho = \sum_{i=1}^{N} \rho_i , \qquad (1.7)$$

we consider the continuity equation along with n-1 species equations for the mass conservation for the gas mixture and each species. The total specific energy E is defined as

$$E = e + \frac{1}{2}\vec{u}^2, \tag{1.8}$$

where

$$e = \sum_{i=1}^{N_s} Y_i e_i \,, \tag{1.9}$$

is the specific internal energy of the gas mixture. In Eq. (1.9), $Y_i = \rho_i / \rho$ is the mass fraction of species *i*, and e_i is the specific internal energy of species *i*. In the calculation, we compute the specific internal energy of the gas mixture from the enthalpy relation and we obtain,

$$e = h - \frac{p}{\rho} = \sum_{i=1}^{N_s} Y_i h_i - \frac{p}{\rho},$$
(1.10)

with

$$h_{i} = \int_{T_{ref}}^{T} C_{pi} dT + h_{fi}$$
(1.11)

where C_{pi} for $i = 1, ..., N_s$ are functions of T only. A database for C_{pi} is available in [4].

Therefore, if the unknown variables (\vec{u} in Eq.(1.2) and (1.5)) at a certain space-time location are known, Eq. (1.10) can be used to calculate *T* by using a Newton iterative procedure.

With the known *T*, *p* is readily obtained by the ideal gas equation or the Noble-Abel equation. The specific heat of individual species C_{pi} appearing in Eq. (1.11) is determined by fourth order polynomials of temperature such as

$$\frac{C_{pi}}{R_u} = a_{i1} + a_{i2}T + a_{i3}T^2 + a_{i4}T^3 + a_{i5}T^4$$
(1.12)

The coefficients of these polynomials are supplied by Gordon and McBride and are valid in a temperature range of 200K to 6000K [4]. The thermodynamic, viscosity, and conductivity data are listed in Appendix A. Next, remembering the mass conservation of species production, the summation of all source terms should be conserved as:

$$\sum_{i=1}^{N} \dot{\omega}_i = 0.$$
 (1.13)

The exchange coupling terms appearing in Eq. (1.3) and Eq. (1.6), $S(\vec{u})$, account for

the particle interaction effects in each conservation equation. First, s_I in the continuity equation is the mass regression rate due to particle evaporation generated by detonating combustion gas. Second, s_{II} and s_{III} (and s_{IV} in 3-d) in the momentum equations are the terms defining the *x* and *y* (and *z*) momentum exchange with the particles per unit volume. Third, the source term s_{IV} (s_V in 3-d) in the energy equation represents the energy exchange and work done by the particles on the gas, such as total energy, heat transfer, and heat of vaporization. Finally, the term, s_i in the species equation is the generation rate of aluminum vapor by evaporation. As a result, the source terms in the continuity, momentum, energy, and species equations could be summarized by taking ensemble averages in each control volume, with an individual particle being labeled by subscript *k*.

$$s_{I} = -\sum_{k} \dot{m}_{k} / V_{i,j}$$
 , (1.14)

$$s_{II,III(IV)} = -\sum_{k} \left[\mathbf{u}_{k} \dot{m}_{k} + m_{k} \frac{d\mathbf{u}_{k}}{dt} \right] / V_{ij} \quad , \qquad (1.15)$$

$$s_{IV(V)} = -\sum_{k} \left[\dot{m}_{k} E_{k} + m_{k} \left(\mathbf{u}_{k} \cdot \frac{d\mathbf{u}_{k}}{dt} \right) + m_{k} c_{l} \frac{dT_{k}}{dt} \right] / V_{i,j} \quad , \tag{1.16}$$

$$s_i = s_i \quad (1.17)$$

where $V_{i,j}$ is the volume involving all particles. \dot{m}_k , $m_k \frac{d\mathbf{u}_k}{dt}$, and $m_k c_l \frac{dI_k}{dt}$ are the rates of the particle mass, momentum and energy change, respectively and will be illustrated in the following sections in detail.

2 DISPERSED PHASE MODEL

In a Lagrangian reference frame, each computational particle, which is individually labeled by subscript k, represents a number of droplets with the same size, position, and velocity. In other words, we use a discrete particle method [5]. Thus, the drop position is given by

$$\frac{d\mathbf{x}_k}{dt} = \mathbf{u}_k \tag{2.1}$$

The regression rate or the rate of particle radius change can be driven by conservation of mass for each particle.

$$\frac{dm_k}{dt} = \frac{d}{dt} \left(\frac{4}{3} \pi \rho_s r_k^3 \right) = -\dot{m}_k \tag{2.2}$$

For modeling the burning of aluminum particles, we employed Khasainov's empirical quasisteady law [6] as:

$$\frac{dr_k}{dt} = -\frac{r_k}{t_b} \left(1 + 0.276 \sqrt{\mathrm{Re}_k} \right)$$
(2.3)

where t_b is the burning time of the aluminum particle given by,

$$t_b = K d_{k,0}^2$$
(2.4)

K is the evaporation rate constant and $d_{k,0}$ is the initial particle diameter. Re_k is the particle Reynolds number which is evaluated by using the relative velocity between the surrounding gas and particle, i.e.,

$$\operatorname{Re}_{k} = \frac{2r_{k} \left| \mathbf{U} - \mathbf{u}_{k} \right| \rho_{g}}{\mu}$$
(2.5)

Next, the instantaneous particle velocity at an arbitrary time is determined by solving the particle momentum equation.

$$m_k \frac{d\mathbf{u}_k}{dt} = m_k \mathbf{g} + D_k \left(\mathbf{U} \right) \left(\mathbf{U} - \mathbf{u}_k \right)$$
(2.6)

where the effects of turbulence on droplet trajectory, i.e., turbulent dispersion, is not considered in this study and the standard gravity of all droplets was used. $D_k(\mathbf{U})$ is the drag function, and is given by

$$D_{k}\left(\mathbf{U}\right) = \frac{1}{2}\pi r_{k}^{2}\rho_{g}C_{D}\left|\mathbf{U}-\mathbf{u}_{k}\right|$$
(2.7)

In Eq. (2.7), the drag coefficient is determined by [7]

$$C_{D} = 2 + \left(C_{D,0} - 2\right) \exp\left(-3.07\sqrt{\gamma}g(\operatorname{Re}_{k})\frac{M}{\operatorname{Re}_{k}}\right) + \frac{h(M)}{\sqrt{\gamma}M}\exp\left(-\operatorname{Re}_{k}/2M\right)(2.8)$$

where $g(\text{Re}_k)$, h(M) are given by,

$$g(\operatorname{Re}_{k}) = \frac{1 + \operatorname{Re}_{k} \left(12.278 + 0.548 \operatorname{Re}_{k}\right)}{1 + 11.278 \operatorname{Re}_{k}}$$
(2.9)

$$h(M) = \frac{5.6}{1+M} + 1.7 \sqrt{\frac{T_k}{T_g}}$$
(2.10)

In addition in Eq. (2.8), $C_{D,0}$ is the standard drag coefficient and is given by,

Considering an energy balance at the particle surface, the rate of particle temperature change can be determined as,

$$m_k c_l \frac{dT_k}{dt} = \frac{dm_k}{dt} L(T_k) + 4\pi r_k^2 \dot{q}_k$$
(2.12)

where $L(T_k)$ is the heat of vaporization, which is constant for the aluminum, c_l is the specific coefficient at constant volume, and \dot{q}_k is the rate of heat conduction over the particle surface per unit area by conduction and radiation.

$$\dot{q}_{k} = \dot{q}_{cond} + \dot{q}_{rad}$$

$$= \frac{k_{g}(T)}{2r_{k}} (T - T_{k}) N u_{k} + \varepsilon \sigma_{b} (T^{4} - T_{k}^{4})$$
(2.13)

Here, $k_g(T)$ is the heat conduction coefficient as a function of the both gas and particle temperature and Nu_k is the Nusselt number given as:

$$Nu_k = 2 + 0.67 \, p \, r^{1/3} \, \mathrm{Re}_k^{1/2} \tag{2.14}$$

In Eq. (2.13), ε is the emissivity of aluminum particles and σ_b (=5.6703 e-8 J/m²K⁴s) is the Stefan-Boltzmann constant.

Accordingly, each aluminum particle exchanges its mass, momentum, and energy with the explosive gas phase by solving Eq.(2.1) ~ (2.14). The amount of aluminum particles was chosen from 1 % to 10% of the initial TNT exploded. The initial particle velocity was assumed to be zero, and the initial particle distribution was taken to be a Rosin-Rammler PDF, where the particles are distributed by referencing an average radius.

$$f = 1 - \exp\left(-\frac{D^{3.5}}{\overline{D}}\right) \tag{2.15}$$

where \overline{D} is the average diameter and f is the accumulated volume. For comparison, we also used a mono-dispersed particle distribution. A particle rebounding from a solid wall is treated with a simple reflection model.

3 COMBUSTION MODEL

After explosion of the TNT, we assume an initial blast where the density, temperature, and pressure are calculated based on a uniform constant volume combustor.

Following this initial explosion, two global reactions are used to convert the carbon dust and carbon monoxide as described in [3].

$$C(s) + \frac{1}{2}O_2 \to CO \tag{3.1}$$

$$CO + \frac{1}{2}O_2 \to CO_2 \tag{3.2}$$

Both reactions are treated as infinitely fast, exothermic combustion. We also assume that the first reaction with the carbon dust, C(s), converts to carbon monoxide, CO, until the source of carbon dust, C(s), or oxygen, O_2 , is depleted. Next, if there is still oxygen remaining, the carbon monoxide burns, producing carbon dioxide, CO_2 . In the calculation, the combustion models for purely TNT explosion without aluminum particles, which was conducted mainly for validation purposes, are solved by using Eq. (3.1) and Eq. (3.2). Detailed derivations to solve the reaction equations are described in Appendix D.

For aluminum combustion, we assume that the aluminum vapor, Al, is solely generated by evaporation. For Al generation, we considered two different types of aluminum combustion: aerobic and anaerobic. In aerobic combution, two global reactions are employed besed on the decomposition temperature [8]. For example, if the gas temperature is lower than the decomposition temperature, T_{dec} , the aluminum vapor burns to aluminum oxide, Al_2O_3 , according to the exothermic reaction.

$$Al + \frac{3}{4}O_2 \rightarrow \frac{1}{2}Al_2O_3, \qquad (3.3)$$

However, if the gas temperature is higher than the decomposition temperature, T_{dec} , the aluminum vapor burns to aluminum monoxide, AlO, according to the endothermic reaction.

$$Al + \frac{1}{2}O_2 \to AlO, \qquad (3.4)$$

Both reations are again treated as infinitly fast.

In an anaerobic reaction, we define the anaerobic combution model as no oxygen reactions for detonaion products behind the flame front. For generated Al gas, we employ two anaerobic aluminum reactions as,

$$Al + \frac{3}{2}H_2O \to \frac{1}{2}Al_2O_3 + \frac{3}{2}H_2$$
(3.5)

$$Al + \frac{3}{2}CO_2 \rightarrow \frac{1}{2}Al_2O_3 + \frac{3}{2}CO$$
 (3.6)

Since each reaction proceeds one after the other based upon the amount of aluminum gas, water vapor, and carbon dioxide in the computational cell, the aluminum oxide is produced depending on whether or not those species are present. Again, both reactions are treated as infinitly fast.

The reaction expressions for the reaction rate in the aerobic case can be calculated as:

$$(\Delta t\dot{r}_{f}) = \min\left[\frac{\rho_{f}}{MW_{f}}, \frac{2\rho_{O_{2}}}{MW_{O_{2}}}\right] \qquad \text{for CO, CO}_{2}, \text{ AlO reaction}$$

$$= \min\left[\frac{\rho_{f}}{MW_{f}}, \frac{4}{3}\frac{\rho_{O_{2}}}{MW_{O_{2}}}\right] \qquad \text{for Al}_{2}O_{3} \text{ reaction} \qquad (3.7)$$

where MW_f is the molecular weight of fuel species f and f represents C(s), CO, or Al. The parenthesis in Eg.(3.7) corresponds to the reaction Eq.(3.3) for the aluminum vapor. In addition, the reaction expressions for the reaction rate in anaerobic case are also calculated as:

$$(\Delta t\dot{r_i}) = \min\left[\frac{\rho_{Al}}{MW_{Al}}, \frac{2}{3}\frac{\rho_{H_2O}}{MW_{H_2O}}\right] \qquad \text{for } H_2\text{O reaction}$$

$$= \min\left[\frac{\rho_{Al}}{MW_{Al}}, \frac{2}{3}\frac{\rho_{CO_2}}{MW_{CO_2}}\right] \qquad \text{for } CO_2 \text{ reaction} \qquad (3.8)$$

where MW_i is the molecular weight of species *i* and *i* represents AL, H_2O , or CO_2 . The first equation in Eq.(3.8) corresponds to the anaerobic reaction between aluminum vapor and water vapor, while the second equation corresponds to the anaerobic reaction between aluminum vapor and carbon dioxide.

After calculating these reaction expressions, the source terms for the species involved in reactions are then described as:

$$\dot{w}_{i} = M W_{i} \sum_{j=1}^{3} \left(v_{ji}^{"} - v_{ji}^{'} \right) \dot{r}_{j}$$
(3.9)

where v'_{ji} and v''_{ji} are the stoichiometric coefficients of reactants and products of species *i* in the *j*th reaction, which are described in Eq. (3.10) for exothermic and Eq. (3.11) for endothermic combustion of aluminum vapor in aerobic reactions, respectively.

$$\mathbf{v}_{ji}^{'} = \begin{bmatrix} 1 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{v}_{ji}^{"} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$
(3.10)
$$\mathbf{v}_{ji}^{'} = \begin{bmatrix} 1 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 1 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{4} & 0 & 0 & 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{v}_{ji}^{"} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$
(3.11)

Based on Eq. (3.9) and aided with Eq. (3.10) and Eq.(3.11), the source term for the species involved in aerobic reactions becomes:

$$\dot{w}_{i} = \begin{cases} -MW_{i}\Delta t\dot{\gamma}_{1} \\ -\frac{1}{2}MW_{2}\Delta t\left(\dot{\gamma}_{1} + \dot{\gamma}_{2} + \frac{3}{2}\dot{\gamma}_{3}\right) \\ MW_{3}\Delta t(\dot{\gamma}_{1} - \dot{\gamma}_{2}) \\ MW_{4}\Delta t\dot{\gamma}_{2} \\ -MW_{5}\Delta t\dot{\gamma}_{3} \\ 0 \\ \frac{1}{2}MW_{7}\Delta t\dot{\gamma}_{3} \end{cases} \quad \text{if } T_{g} < T_{dec} \qquad (3.12)$$

$$\dot{w}_{i} = \begin{cases} -MW_{1}\Delta t\dot{\gamma}_{C(s)} \\ -\frac{1}{2}MW_{2}\Delta t(\dot{\gamma}_{C(s)} + \dot{\gamma}_{cO} + \dot{\gamma}_{Al}) \\ MW_{3}\Delta t(\dot{\gamma}_{C(s)} - \dot{\gamma}_{CO}) \\ MW_{4}\Delta t\dot{\gamma}_{CO} \\ -MW_{5}\Delta t\dot{\gamma}_{Al} \\ MW_{6}\Delta t\dot{\gamma}_{Al} \\ 0 \\ 0 \end{cases} \quad \text{if } T_{g} > T_{dec} \qquad (3.13)$$

where the species involved in chemical reaction are C(S), O_2 , CO, CO_2 , Al, AlO, and Al₂O₃ in the above equations, respectively. Since each reaction is proceed one after another depending on the amount of the oxygen in the computational cell, the oxygen is a controlling key for the reactions.

On the other hand, in Eq. (3.5) and (3.6), the stoichiometric coefficients of reactants and products of species *i* in the *j*th reaction, are described in Eq. (3.14) for the anaerobic and exothermic combustion of aluminum vapor.

$$\mathbf{v}_{ji}^{'} = \begin{bmatrix} 0, & 0, & 1, & 0, & \frac{3}{2}, & 0\\ 0, & \frac{3}{2}, & 1, & 0, & 0, & 0 \end{bmatrix}, \quad \mathbf{v}_{ji}^{'} = \begin{bmatrix} 0, & 0, & 0, & \frac{1}{2}, & 0, & \frac{3}{2}\\ \frac{3}{2}, & 0, & 0, & \frac{1}{2}, & 0, & 0 \end{bmatrix} (3.14)$$

Base on the Eq. (3.9) and aided with Eq. (3.14), the source term for the species involved in this reaction becomes:

$$\dot{w}_{i} = \begin{cases} \frac{3}{2} M W_{1} \Delta t \dot{\gamma}_{2} \\ -\frac{3}{2} M W_{2} \Delta t \dot{\gamma}_{2} \\ -M W_{3} \Delta t (\dot{\gamma}_{1} + \dot{\gamma}_{2}) \\ \frac{1}{2} M W_{4} \Delta t (\dot{\gamma}_{1} + \dot{\gamma}_{2}) \\ -\frac{3}{2} M W_{5} \Delta t \dot{\gamma}_{1} \\ \frac{3}{2} M W_{6} \Delta t \dot{\gamma}_{1} \end{cases}$$
(3.15)

where the species involved in anaerobic chemical reactions are CO, CO₂, Al, Al₂O₃, H₂O and H₂ in the above equations, respectively. Again, each reaction proceeds one after the other depending on the bonding energy of the chemical compounds. Treated as a high temperature and pressure explosive gas, the Noble-Abel equation of state is recommended [3], which considers the effect of finite volume molecules, as:

$$P = \frac{\rho RT}{1-an} \tag{3.16}$$

where a, 25 or 15 cm^3/mol , is empirically determined and n is the molar density of the gas.

INITIAL CONDITIONS AND KEYWORD SAMPLE

Initial conditions such as density, pressure, and temperature in the initial blast region are set from the first fireball values based on a constant volume well-stirred reactor calculation, and conditions away from the initial blast region are set to the ambient conditions. Detailed thermodynamic conditions and species mass fractions are listed in Table 1~3. For aluminum particles which are initially distributed by a Rosin-Rommler or mono-dispersed distribution, zero or constant velocities are assumed with the same thermodynamic initial conditions as the explosive products. Since the melting temperature of an aluminum particle is 933K, the ignition temperature of the aluminum particles in the basic case was set to 1000K. The initial amount of aluminum particles was changed from 1% to 10% of TNT.

Initial conditions for a constant volume explosion of 2.12 Kg of TNT.

Table 1. Initial charge of TNT		
Amount of TNT	2.12 Kg	
Mole TNT	9.334	
Volume TNT	$1,285 \text{ cm}^3$	
Radius of blast	11.1 cm	
Volume of blast	$5,729 \text{ cm}^3$	

Table 2. Gas initial conditions

	Mole	Density(mol/cm ³)
O ₂	0.0489	8.532×10 ⁻⁶
N ₂	0.1838	3.208×10 ⁻⁵
Temperature	300.0 K	
Pressure	1013 bar	
Molar density	$4.061 \times 10^{-5} \text{ mol/cm}^{3}$	
Molecular weight	28.85 gm/mol	

Table 3. Gas final conditions

	Mole	Density(mol/cm ³)
C(s)	32.57	5.686×10 ⁻³
O ₂	0	0
N ₂	14.18	2.476×10 ⁻³
H ₂ O	23.33	4.073×10 ⁻³
СО	32.77	5.720×10 ⁻³
CO ₂	0	0
Temperature	3501 K	
Pressure	4,376 bar	
Molar density	$12.27 \times 10^{-3} \text{ mol/cm}^{-3}$	
Molecular weight	24.78	

ELEMENTS H O C AL N END SPECIES C(S) 02 CO CO2 AL ALO AL203(S) H20 H2 N2 END THERMO END

*** Chemistry input file for tbx key word file

*KEYWORD *TITLE Tbxp_3d \$ \$ +CESE_CONTROL_SOLVER iflow \$ icese igeom eqtp 0 1 3 0 *CESE_CONTROL_TIMESTEP \$ iddt cfl dtint 1 0.03 2.0e-8 *CESE_CONTROL_LIMITER ialfa \$ idlmt beta epsr 0 2.0 1.0 0.0 *CONTROL_TERMINATION endeng \$ endtim endcyc dtmin endmas 40.0 900000 \$ \$ \$ Setup the boundary conditions for fluid \$ \$ Symmetry BC_1 (bottom and left wall) \$ *CESE_BC_REFLECTIVE_SET ssid \$ 1 \$ \$ Reflect BC_2 (top and right) \$ +CESE_BC_SOLID_WALL_SET \$ ssid 2 \$ ۰ *CHEMISTRY_CONTROL_TBX \$ model_id npar 10 1 \$ *CHEMISTRY MODEL \$ model_id jacsel errlim -10 0.0 1 tbxp.inp thermtbx.dat tran.dat ۰ \$ the global domain: embient condition with air *CHEMISTRY_COMPOSITION \$ comp_id model_id 11 10 \$ molcon species .04612 02 .17341 N2 \$ the explosive domain *CHEMISTRY_COMPOSITION \$ comp_id model_id 12 10 species molcon \$ C(S) 5841.86 5877.73 C0 4184.54 H20 2543.37 N2 *CESE_INITIAL_CHEM \$ model_id comp_id 10 11

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$INITIAL CONDITIONS
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                                           0.3
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                   z_org
                          x_vel
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*CESE_MAT_GAS
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                     c2
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      1
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*CESE_EOS_IDEAL_GAS
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   eosid
             cv
      1
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5
$ Handle output of state and restart data
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*DATABASE_BINARY_D3PLOT
$ dt/cycl
            lcdt
                   beam
                          npltc
   1.0e-8
                      0
*DATABASE BINARY D3DUMP
$ dt/cycl lcdt
                   beam
                          npltc
$ dt/cycl
   10000
$
*INCLUDE
det_3d_mesh_ts.k
*CONTROL_STRUCTURED
*END
```

*** Keyword file for tbx with aluminum particles. Sample keyword files, including 2-D and 3-D versions without particles are available at ftp/anonymous/outgoing/ksim/examples/tbx.

RESULTS

INITIAL BLAST SIMULATION

Spherical geometry with a radius of 173 cm is considered for a one-dimensional calculation with a blast radius of 11.1 cm. Figure 1 shows the consecutive snapshots for the main flow properties of the initial blast wave propagation after TNT explosion at consecutive times. At an earlier time instant, 50 μ s in Figure 1a, the flame and shock wave are coincidently propagating without any separation, which is still a detonation wave. As time progress further, the flame is detached from the shock wave and the gap between waves are significantly increased by 1050 μ s. In addition, the reaction zone is confined at the thin layer due to the poor mixing between combustible detonation products and air. As the blast wave expands, the initial pressure of 4367 bar reduces quickly to 40 bar at a radius of 50cm (see Figure 1b). The same phenomenon can be also seen in density propagation profiles in Figure 1d. Even though the density was extremely high in the initial blast volume, at about 40 cm, the maximum value falls to less than 10 Kg/m³. As enough time progresses, both the density and pressure in the original blast volume decrease below the ambient values because of over-expansion. Due to this expansion, the velocity becomes negative between the shock front and the original blast volume. All trends match well with Schwer's results in [9].



Figure 1 Initial blast wave propagation, R_b=11.1cm, W_{TNT}=2.12 kg: a) temperature, b) pressure, c) velocity, and d) density



Figure 2 Loci curves of the shock front and flame front

Figure 2 shows the propagation of the shock wave front and flame front in a onedimensional domain. The separation between the shock wave and the flame front begins at about 50 cm from the blast origin. After this point, the initial detonation wave becomes a fast combustion wave, which is not premixed due to air mixing. It is at this position that the extinguishing process starts, and the mixing process among carbon dust, C(s) and CO and oxygen is the dominant mechanism for combustion.

STEADY SIMULATION WITHOUT ALUMINUM

In this two-dimensional steady simulation, one of the axisymmetric planes, which has dimensions of 173 cm(axial direction) \times 173 cm (radial direction), was used with the same blast radius as the one-dimensional case shown in Figure 1.



Figure 3 Geometry and pressure trace locations for axisymmetric coordinates: P1(0.37cm, 0.37cm), P2(0.37cm, 86.5cm), P3(0.37cm, 172.7cm), P4(86.5cm, 0.37cm), P5(86.5cm, 86.5cm), P6(86.5cm, 172.7cm), P7(172.7cm, 0.37cm), P8(172.7cm, 86.5cm), v P9(172.7cm, 172.7cm). In addition, to compare the overpressure history profiles in time with the previous results[4], we selected 8 different positions as close as possible to the wall surface and one center position shown in Figure 3. For the simulation, we used a TNT explosive of 2.12kg at the center of cylinder (or sphere) in the confined area [9].

To examine the mixing process, we conducted the long time calculation about 50 ms after SOC (start of calculation). Figure 4 shows consecutive snapshots of the temperature distributions at different time instants. In the initial stage, the blast seems to propagate symmetrically until the shock wave hits the side walls (Figure 4a and 4b). After the shock wave reflects from the wall (see Figure 4c) at time 5ms after SOC, it is difficult to detect the shock front and instead, the flame starts to become a random mixing process. From 10 ms to 20 ms (refer in Figure 4d~f), the flame develops more random patterns and reaches very high temperatures. After this period, the flame gets weaker and weaker as shown in Figure 4g~i. At 50 ms after SOC, the total area of the red spots was recognizably reduced from the previous period, indicating that the extinguishing of the flame proceeds to a certain degree by this time instant.



Figure 4 Snapshots of the temperature distributions at different times.

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