NUMERICAL SIMULATION OF AFTERBURNING OF THERMOBARIC EXPLOSIVE PRODUCTS IN AIR

C.-K. Kim[1], J.-S. Hwang[2] and K.-S. Im[3]

[1,2]*Explosive Trains and Gun Propellant Team, Agency for Defense Development ,Yuseong P.O. Box 35-5, Daejeon, Republic of Korea*
[3]*Argonne National Laboratory, Argonne, Illinois 60439, USA*

To predict the blast performance of thermobaric warhead, numerical modeling of secondary burning after detonation of thermobaric explosives is investigated. We select TNT containing small quantity of aluminum as a candidate thermobaric explosive. The combustion process is modeled by the fast reaction for gas and aluminum vapor and the finite-rate burning for aluminum particle. The simulations are performed by the space-time Conservation Element and Solution Element, or CESE method, which is a state-of-art CFD technology to solve conservation laws.

INTRODUCTION

Compared to conventional high explosives, thermobaric explosives have enhanced thermal and blast effects. They are explosives with oxygen-deficient composition containing metal particles such as aluminum and magnesium. Thermobaric effects are obtained by long duration overpressure and heat due to the afterburning of detonation products with air. Because the afterburning process is controlled by turbulent mixing and combustion with air after detonation or dispersion by bursting charge, even the identical explosive composition may yield different thermal and blast performance with targets. Therefore, we need to understand the afterburning mechanism exactly to design warhead optimally for various operational environments.

As a preliminary stage for this purpose, present study is focused on the numerical simulation of afterburning of detonation products with air in axi-symmetric enclosure. We select TNT containing small quantity of aluminum as a candidate of thermobaric explosive. Afterburning is very complex process containing the blast propagation from initial detonation products in high pressure and temperature, shock reflections at the wall and their interaction, turbulent mixing with air, two-phase flow effect due to particles, and combustion. The combustion process is modeled by the fast reaction for

gas and aluminum vapor and the finite-rate burning for aluminum particle. The simulations are performed by the space-time Conservation Element and Solution Element, or CE/SE method, which is a state-of-the art CFD technology to solve conservation laws.

Through numerical simulations, the characteristics of the initial blast wave propagation and afterburning process are presented.

GOVERNING EQUATIONS

The conservation equations governing unsteady, the explosive detonating gas with exothermic and aluminum particle combustions could be a 2-dimensional Euler equation in the axisymmetric coordinate system. The combined vector form of those governing equations is summarized as:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{E}(\mathbf{U})}{\partial x}+\frac{\partial \mathbf{F}(\mathbf{U})}{\partial y}=\mathbf{G}(\mathbf{U})+\mathbf{S}(\mathbf{U})+\mathbf{W}(\mathbf{U}) \tag{1}$$

where x, y≥0, and t are the axial and radial coordinates, and time, respectively. The primitive flow variable **U**, the flux vectors, **E(U**) and **F**(**U**) are described as:

$$\mathbf{U} = \left[\rho,\rho u,\rho v,\rho E,\rho_1,\rho_2,\rho_3\ldots,\rho_{n-1}\right]^T, \tag{2a}$$

$$\mathbf{E}(\mathbf{U}) = \left[\rho u,\rho u^2+p,\rho uv,(\rho E+p)u,,\rho_1 u,\rho_2 u,\rho_3 u\ldots,\rho_{n-1}u\right]^T, \tag{2b}$$

$$\mathbf{F}(\mathbf{U}) = \left[\rho v,\rho u\mathrm{v},\rho v^2+p,(\rho E+p)v,,\rho_1 v,\rho_2 v,\rho_3 v\ldots,\rho_{n-1}v\right]^T. \tag{2c}$$

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 density of species i, which are considered in exothermic and aluminum particle combustion. The sources terms, **G**(**U**), **S**(**U**), and **W**(**U**) due to the axisymmetric geometry, the exchange coupling terms between the explosive gas and solid aluminum particles, and the chemical reaction are also described as:

$$\mathbf{G}(\mathbf{U}) = -\frac{1}{y}\left[\rho v,\rho u\mathrm{v},\rho v^2,(\rho E+p)v,,\rho_1 v,\rho_2 v,\rho_3 v\ldots,\rho_{n-1}v\right]^T, \tag{2d}$$

$$\mathbf{S}(\mathbf{U}) = \left[s_I, s_{II}, s_{III}, s_{IV}, 0, 0, 0, \ldots, s_i, \ldots, 0\right]^T \tag{2e}$$

$$\mathbf{W}(\mathbf{U}) = \left[0, 0, 0, 0, \dot{\omega}_1, \dot{\omega}_2, \dot{\omega}_3 \ldots, \dot{\omega}_{n-1}\right]^T, \tag{2f}$$

where s_I, s_{II}, s_{III}, s_{IV}, and s_i are the exchange terms representing mass, momentums, energy, and generation of the aluminum gas due to the evaporation. The source terms $\dot{\omega}_i$ for $i=1,2,\cdots,n-1$ in the species equations are the production rates of species i of chemical reactions involved.

The exchange coupling terms appearing in Eq. (2e), **S**(**U**), account for the particle interaction effects on each conservative equation. First, mass regression rate, s_I, is considered in the continuity equation because of the particle evaporation due to the exothermic combustion. Second, s_{II} and s_{III} in the momentum equations are the terms defining the *x* and *y* momentum exchange with the particles per unit volume. Third, the source term s_{IV} in energy equation represents the energy exchange and work done by the particles to the gas such as total energy, heat transfer, and heat of vaporization. Finally, the term, s_i, in species equation is representing the generation rate of the aluminum vapor by evaporation. As a result, the source terms in continuity, momentum, energy, and species equation could be summarized by taking ensemble averages in each control volume if an individual particle is labeled by subscript *k*.

$$s_I = -\sum_k \dot{m}_k / V_{i,j} \quad , \tag{3}$$

$$s_{II,III} = -\sum_k \left[\mathbf{u}_k \dot{m}_k + m_k \frac{d\mathbf{u}_k}{dt} \right] \Big/ V_{i,j} \quad , \tag{4}$$

$$s_{IV} = -\sum_k \left[\dot{m}_k E_k + m_k \left(\mathbf{u}_k \cdot \frac{d\mathbf{u}_k}{dt} \right) + m_k c_l \frac{dT_k}{dt} \right] \Big/ V_{i,j} \quad , \tag{5}$$

$$s_i = -s_I \quad . \tag{6}$$

where $V_{i,j}$ is the volume involved all particles and other terms in the above will be illustrated in the following sections in detail.

COMBUSTION MODELS

After detonation of the TNT, we assume the initial blast where the density, temperature, and pressure are calculated based on the uniform constant volume combustor. Following this initial explosion, two global reactions are sued to convert the carbon dust and carbon monoxide as described in [Schwer and Kailasanath,2002].

$$C(s) + \frac{1}{2} O_2 \rightarrow CO \quad , \; CO + \frac{1}{2} O_2 \rightarrow CO_2 \tag{7}$$

Here, both reations are treated as infinitly fast, exothermi combustion. we also assume that the first, the carbon dust, *C(s)*, converts to carbon monoxide, *CO*, until the providing of the carbon dust, *C(s)*, or oxygen, O_2, is depleted and next, if there is still oxygen remained, the carbon monoxide burn to carbon dioxide, CO_2. For the aluminum combustion, we assume that the aluminum vapor, Al, is solely generated by evaporation. With the Al generation, again, two global reactions are employed besed on the decomposition temperature [Hayashi, 2006]. If the gas temperature is lower than the

decomposition temperature, T_{dec}, the aluminum vapor burn to the aluminum oxide, Al_2O_3 according to the exothermic reaction.

$$Al + \frac{3}{4}O_2 \rightarrow \frac{1}{2}Al_2O_3 \quad , \tag{8}$$

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

$$Al + \frac{1}{2}O_2 \rightarrow AlO \quad , \tag{9}$$

Again, both reations are treated as infinitly fast. The reaction expressions for the reaction rate used as:

$$(\Delta t\dot{r}_f) = \min\left[\frac{\rho_f}{MW_f}, \frac{2\rho_{O_2}}{MW_{O_2}}\left(\frac{4}{3}\frac{\rho_{O_2}}{MW_{O_2}}\right)\right] \tag{10}$$

where MW_f is the molecular weight of species and *f* represents *C(s)*, *CO*, or *Al*. The parenthesis in Eg.(10) stands for the reaction Eq.(8), (9) for the aluminum. The source term for the species involved in reactions also given as:

$$\dot{w}_i = MW_i \sum_{j=1}^{2}\left(\nu''_{ji} - \nu'_{ji}\right)\dot{r}_j \tag{11}$$

Here, ν'_{ji} and ν''_{ji} are the stoichiometric coefficients of reactants and products of species i in the j th reaction.

Treating as the high temperature and pressure explosive gas, the Nobel-Able equation of state is recommended, which considers the effect of finite volume molecules, as:

$$P = \frac{\rho RT}{1\text{-}an} \tag{12}$$

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

DISPERSED PHASE EQUATIONS

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 used discrete particle method [Dukowicz, 1980]. Thus, the drop position is given by

$$\frac{d\mathbf{x}_k}{dt} = \mathbf{u}_k \tag{13}$$

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

$$\frac{dm_k}{dt} = \frac{d}{dt}\left(\frac{4}{3}\pi\rho_s r_k^3\right) = -\dot{m}_k \tag{14}$$

For modeling the burning of aluminum particles, we employed Khasainov's empirical quasisteady law [4] as:

$$\frac{dr_k}{dt} = -\frac{r_k}{t_b}\left(1 + 0.276\sqrt{\mathrm{Re}_k}\right) \tag{15}$$

where t_b is the burning time of the aluminum particle given as [4],

$$t_b = Kd_{k,0}^2 \tag{16}$$

Here, 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 relative velocity between the surrounding gas and particle, i.e.,

$$\mathrm{Re}_k = \frac{2r_k\left|\mathbf{U} - \mathbf{u}_k\right|\rho_g}{\mu} \tag{17}$$

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

$$m_k\frac{d\mathbf{u}_k}{dt} = m_k\mathbf{g} + D_k\left(\mathbf{U}\right)\left(\mathbf{U} - \mathbf{u}_k\right) \tag{18}$$

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

$$D_k\left(\mathbf{U}\right) = \frac{1}{2}\pi r_k^2\rho_g C_D\left|\mathbf{U} - \mathbf{u}_k\right| \tag{19}$$

In Eq. (19), the drag coefficient is determined by [2]

$$C_D = 2 + \left(C_{D,0} - 2\right)\exp\left(-3.07\sqrt{\gamma}\,g(\mathrm{Re}_k)\frac{\mathrm{M}}{\mathrm{Re}_k}\right) + \frac{h(\mathrm{M})}{\sqrt{\gamma}\mathrm{M}}\exp\left(-\mathrm{Re}_k/2\mathrm{M}\right) \tag{20}$$

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

$$m_k c_l \frac{dT_k}{dt} = \frac{dm_k}{dt} L(T_k) + 4\pi r_k^2 \dot{q}_k \tag{21}$$

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 to the particle surface per unit area.

$$\dot{q}_k = \frac{k_g(T)}{2r_k}\left(T - T_k\right) Nu_k \tag{22}$$

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:

$$Nu_k = 2 + 0.67\, pr^{1/3}\, \mathrm{Re}_k^{1/2} \tag{23}$$

Accordingly, each aluminum particle exchanges its mass, momentum, and energy with the explosive gas phase by solving Eq.(13) ~ (23). The amount of the aluminum particle was considered as 10% of the initial TNT exploded. The initial particle velocity was assumed zero velocity and the initial particle distribution was considered as a Rosin-Rammler, where the particles are distributed by referencing an average radius.

$$f = 1 - \exp\left(-\frac{D^{3.5}}{\overline{D}}\right) \tag{24}$$

where $\overline{D}$ is the average diameter and f is the accumulated volume. The particle rebounding from the wall was treated with a simple reflection model.

NUMERICAL METHOD

The space-time Conservation Element Solution Element (CESE) method [5, 6] was applied to solve the reacting flow. The space-time CESE method is a high-resolution and genuinely multidimensional method for solving conservation laws. It has a solid foundation in physics and yet is simple in mathematics. Its nontraditional features are: (i) a unified treatment of space and time, (ii) the introduction of conservation element (CE) and solution element (SE) as the vehicles for enforcing space-time flux conservation, and (iii) a time marching strategy that has a space-time staggered stencil at its core and, as such, can capture shocks without using Riemann solvers.

RESULTS

For the simulation, we select the case of TNT (2.12kg) detonation at the center of cylinder of a radius of 173cm and a length of 346cm as [1]. Then, the computation domain is 173cm ×173cm by symmetry. As previously mentioned, the simulation is initialized by defining a blast volume. The initial blast radius is assumed by 11.1cm. Total amount of the aluminum particles that is uniformly distributed in the initial blast area was approximately 10 % (200g) to the TNT.

Figure 1 shows the initial blast wave propagation after TNT detonation without aluminum, From the temperature profile, we can see that the reaction zone is confined at the thin layer behind the blast front 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 about radius of 50cm.

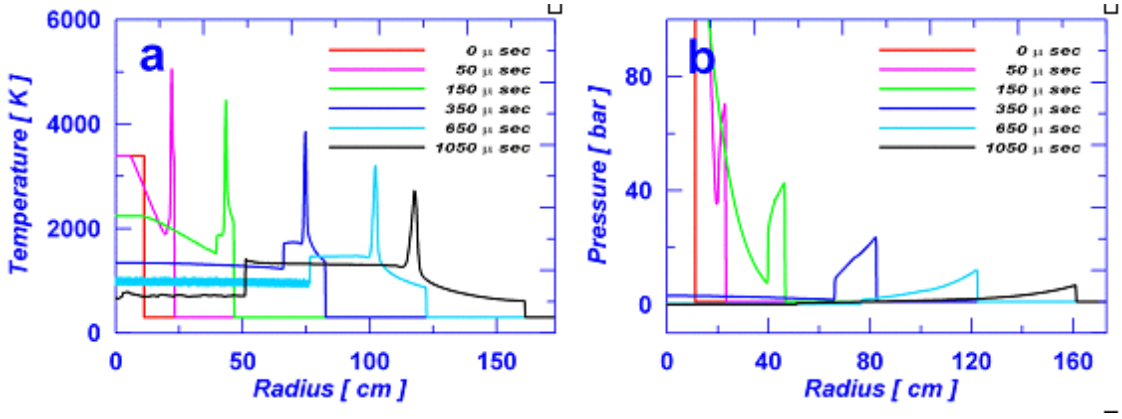

Figure 1. Initial blast wave propagation, R_b=11.1cm, W_{TNT}=2.12 kg: a) temperature, b) pressure

Figure 2 illustrates the time evolution snapshots of the TNT explosion with aluminum particles. Initially, Rosin-Rammler distribution that has an average mean diameter of 10 μm was assumed with zero velocity for all particles. The pressure wave symmetrically propagates to the outward, which is quite similar to that of no particle case, but the mass fraction of the aluminum vapor shows very different trend such that most vapor mass is distributed near the bottom wall. However, it is interesting to see the symmetric distribution of the AlO species. Since the production rate of the AlO species depends on the amount of the oxygen remaining in the combustion gas, its distribution is not directly related to the aluminum vapor but the remaining oxygen. It is also note that at earlier stage of the detonation propagation, the Al_2O_3 species is not produced yet, which will be demonstrated our next study.

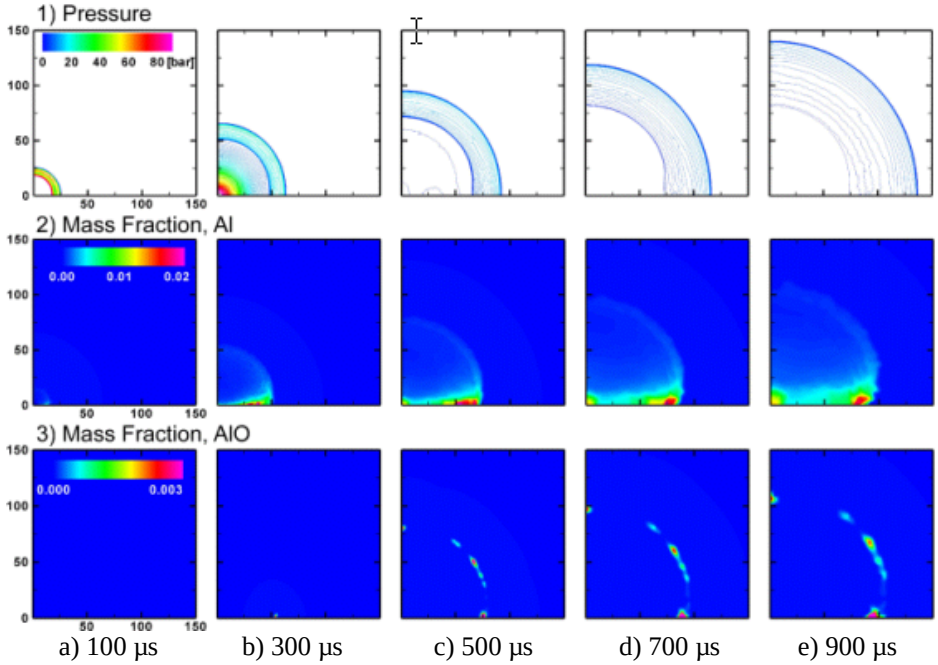

Figure 2. Progressive propagation of TNT explosion with aluminum particles: 1) pressure; 2) mass fraction of Al species; and 3) mass fraction of AlO species.

CONCLUSIONS

To predict the blast performance of thermobaric warhead, numerical modeling of secondary burning after detonation of thermobaric explosives containing aluminum particles was presented. The numerical simulation was conducted using the space-time CESE method.

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