A Modified Mixture Rules for Mie-Grüneisen Mixture Model

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Abstract. The Mie-Grüneisen mixture model can be conveniently used in multicomponent flow. However, the mixture rules in the original model can’t distinguish components at the interface. That cause abnormal transition near the interface. To solve this problem, a modified mixture rules which based on mass fraction is used here. And three non-conservative equations are added here to keep the pressure equilibrium condition. Comparing with the original mixture rules, the transition form at the interface is revised and the curve of sound speed is optimized. With the help of the modified rules, the times steps in calculation are reduced. Moreover, for spherical coordinate system, the modified mixture rules not only save steps but also get more accurate solution.

1 Introduction

Up to now, the multicomponent Riemann problem has been studied for a long time [1]. The oscillation control of interface is a key process in calculation all the time [2], [3]. For general type equations of states (EOS), which is always written in a Mie-Grüneisen form [4], [5], the treatment of interface is more difficult because the approximate Riemann solver is hard to be adopt for such a complex EOS.

Without the approximate Riemann solver, the fluid field is always considered as a whole mixture [3]. And each relative parameter is considered as a particular parameter for mixture. These parameters for mixture are always a weighted sum of each component. However, the parameters are not summed in a same style. The mixture rules of the sum, plays an important role in calculation.

There is variety of ways to define the mixture rules for parameters. An efficient way is connecting each component to the mixture by volume fraction. This technique took effects on two models. One is the model of Saurel-Abgrall [6], which includes three Euler equations for each component and transport equations for each interface. Another model is a five-equations model provided by Allaire [7]. This model contains Euler equations for mixture and mass conservation equations for components, as well as transport equations for interface. Both the two models have a similar procedure: evaluating the pressure at interface by a pressure closer, which represents a relationship about the pressure at two sides. Unlike other difference equations, the pressure closer is always solved by a numerical approximation, which makes the calculation complex.

Other ways are also used to define the parameters of mixture. Henry de Frahan [8] regard the parameters as a function of mass fraction and specific heats ratio $\gamma$. To prevent the oscillations, a DG procedure is used in this approach. Shukla[9] created a level set function $\phi$. Then the relationship among different components is constructed with the help of $\phi$. Recently, Garrick [10] established mixture model in terms of volume fraction and then reconstructed the interface according a THINC procedure.

No matter the volume fraction model of Saurel-Abgrall and Allaire, nor other above-mention models, it is necessary to use additional techniques, such as pressure closer, interface reconstruction, and so on. Comparing with these models, a Mie-Grüneisen mixture model of Shyue[4],[5], can solve the multi-component problem without any other additional technique. And the pressure is calculated directly by EOS, rather than pressure closer at interface. However, the numerical stability of interface relies much on the parameters transition.

The current Mie-Grüneisen mixture model also chooses volume fraction as the connection of components. In contrast, mass fraction is seldom used in the mixture models. It is testified by R. Abgrall that the traditional rules of mass fraction always lack the stability at interface [2]. To replace volume fraction with mass fraction, the mixture rules need to be seriously constructed.

In this article, the mixture rules of original Mie-Grüneisen mixture model are modified here. To avoid pressure oscillation, the unsteady traditional rules of mass fraction are abandoned here. The modified rules preserve the equilibrium condition in original model and avoid the oscillation. The main advantage of the modified rules is that the time steps in calculation are obviously reduced due to the optimization of sound speed. This advantage is then testified by examples.
2 Mie-Grüneisen Mixture Rules

2.1 Equations System

For the compressible fluids, conservative Euler equation is applied to be the basic governing equation:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (1)$$

where $U$ is vector of conservative variables, and $F$ are fluxes. They can be written as:

$$U = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho E + p u \\ \rho E \end{bmatrix}$$

where $E$ is total energy, and can be described by an addition of internal energy $e$ and kinetic energy:

$$E = e + \frac{1}{2} u^2$$

besides the Euler equations (1), a supplement of EOS is needed here:

$$p - p_{ref}(\rho) = \rho \Gamma (e - e_{ref}(\rho)) \quad (2)$$

(2) is the Mie-Grüneisen equations, in which there are three thermodynamic parameters: $\Gamma$, $p_{ref}$, $e_{ref}$. $\Gamma$ is the Grüneisen parameter, $p_{ref}$ and $e_{ref}$ are pressure and inner energy of reference states. The three parameters are calculated by three non-conservative transport equations:

$$\frac{\partial}{\partial t} \begin{bmatrix} \frac{\Gamma}{\Gamma} \\ \frac{\Gamma}{p_{ref}} \\ \frac{\Gamma}{e_{ref}} \end{bmatrix} + u \frac{\partial}{\partial x} \begin{bmatrix} \frac{\Gamma}{\Gamma} \\ \frac{\Gamma}{p_{ref}} \\ \frac{\Gamma}{e_{ref}} \end{bmatrix} + p \frac{\partial \varphi}{\partial x} \begin{bmatrix} \rho \\ \varphi \\ \varphi \\ \varphi \end{bmatrix} = 0 \quad (3)$$

where the symbols $\varphi$, $\varphi$ and $\varphi$ denote the derivative functions of the items $\Gamma$, $p_{ref}$, $e_{ref}$, respectively. For multi-component problem, the transportation of interface is also needed to be considered. In the original Mie-Grüneisen mixture model, the transport equations of $m$-components flow are related to volume fraction:

$$\frac{\partial z_i}{\partial t} + u \frac{\partial z_i}{\partial x} = 0 \quad (i = 1, \ldots, m-1) \quad (4)$$

where $z_i$ denote the volume fraction. The transport equations can be also related to mass fraction:

$$\frac{\partial (\rho y_i)}{\partial t} + \frac{\partial (\rho y_i u)}{\partial x} = 0 \quad (i = 1, \ldots, m-1) \quad (5)$$

$y_i$ is the mass fraction. Either (4) or (5) is enough for the solver of Mie-Grüneisen mixture model. Between (4) or (5), (5) is always replaced by (4) due to the lack of mixture rules which can control the pressure oscillation.

2.2 R. Abgrall’s Rules of Mass Fraction

In the multi-component problem, the interface is always considered as a diffused region where different fluid components coexist together. The parameters of the mixture are deduced according to the mixture rules. In that case, the numerical stability of the parameters relies much on the mixture rules.

The mass fraction, coupled with equations as (5), has been already tested by R. Abgrall many years ago [2]. However, the traditional mixture rules of $y_i$ in calculation are not coupled with the Mie-Grüneisen mixture model. Fortunately, oscillations are found at interface. In the traditional mixture rules of R. Abgrall, the density of each component $\rho y_i$ is obtained by (5), then $\rho y_i$ can be directly used to compute the parameters $1/\Gamma$, $p_{ref}/\Gamma$ and $pe_{ref}$ for each component. In fact, these three parameters strictly computed by $\rho y_i$ cannot satisfy the pressure equilibrium. If one uses these parameters to deduce the pressure, it is hard to control the oscillation. The oscillation of pressure finally causes the abandon of mass fraction.

Comparing with $y_i$, the volume fraction $z_i$ is expressed in a non-conservative transport form. In non-conservative form, the pressure equilibrium becomes an implicit condition [2]. The mixture rules of $z_i$ guarantees pressure stable but lose the ability to calculate the density of component.

2.3 Original $z_i$ Mixture Rules

Then our attentions are transferred back to the original mixture rules of Mie-Grüneisen mixture model, which based on volume fraction $z_i$. In the original rules, the flow mixture is considered as an entire mixture with uniform parameters (including $\rho$, $u$, $p$, $E$, $\Gamma$, $p_{ref}$ and $e_{ref}$). For examples, the mixture density is $\rho$, the density of the first, second, component is also $\rho$. The parameters for every component are considered the same as the mixture.

According to this mixture rules, all parameters of the mixture are taken as parameters for components except for $z_i$. So the items $\varphi$, $\varphi$ and $\varphi$ are as following:

$$\varphi = z_1 \left( \frac{1}{\Gamma_1} \right)^{\gamma} + z_2 \left( \frac{1}{\Gamma_2} \right)^{\gamma} + \cdots + z_m \left( \frac{1}{\Gamma_m} \right)^{\gamma} \quad (6)$$

$$\varphi = z_1 \left( \frac{p_{ref1}}{1/\Gamma_1} \right)^{\gamma} + z_2 \left( \frac{p_{ref2}}{1/\Gamma_2} \right)^{\gamma} + \cdots + z_m \left( \frac{p_{refm}}{1/\Gamma_m} \right)^{\gamma}$$

$$\varphi = z_1 \left( \frac{pe_{ref1}}{1/\Gamma_1} \right)^{\gamma} + z_2 \left( \frac{pe_{ref2}}{1/\Gamma_2} \right)^{\gamma} + \cdots + z_m \left( \frac{pe_{refm}}{1/\Gamma_m} \right)^{\gamma}$$

where the corner symbols denotes the number of the component. It can be noticed in (6) that the items $\varphi$, $\varphi$ and $\varphi$ are functions of $\rho$ and $z_i$. Except for these three items, other parameters all represent which of mixture.

The mixture pressure $p$ is calculated as:

$$p = \frac{\rho E - \frac{1}{2} \rho u^2 - \rho e_{ref} + \rho e_{ref}}{1/\Gamma} \quad (7)$$

as the pressure equilibrium is implicitly considered in (3), the expressions (7) can avoid oscillation.
With the help of mixture rules as (6), the equations system of Mie-Grüneisen mixture model can be well established. It evolves conservative equations (1) and non-conservative equations (3), as well as transport equations (4) or (5).

2.4 Modified \( y_i \) Mixture Rules

Now the mixture rules in terms of \( z_i \) are used in current Mie-Grüneisen mixture model. It must be noticed that the items \( \phi, \varphi \) and \( \psi \) are not theoretically correct. These three items are actually the functions of \( \rho y_i \) rather than \( \rho \). So it is significant to establish new mixture rules of \( \rho y_i \).

It is emphasized here that we only make a change to the mixture rules, so equations (3) are preserved. Thanks to the pressure equilibrium conditions in (3), the modified mixture rules can avoid oscillation. Comparing with R. Abgrall’s traditional rules of mass fraction, the pressure is deduced by \( \Gamma, p_{\text{ref}} \) and \( e_{\text{ref}} \) rather than \( \rho y_i \). As the calculation of \( \Gamma, p_{\text{ref}} \) and \( e_{\text{ref}} \) is based on pressure equilibrium, there is no oscillation in the modified rules.

For the relative parameters \( \rho, u, p, E, \Gamma, p_{\text{ref}} \) and \( e_{\text{ref}} \), we only need to consider the parameters of mixture. For derivative items \( \phi, \varphi \) and \( \psi \), if the expression of EOS for components is different from the adjacent component, the values of \( \phi, \varphi \) and \( \psi \) would be affected due to the ignorance of individual EOS for each component. So we must consider their expressions and values in components.

Here we consider the differential of \( 1/\Gamma \) first:

\[
d(1/\Gamma) = (1/(\Gamma_1^{y_1}) + (1/(\Gamma_2^{y_2})) + \cdots + (1/(\Gamma_n^{y_n})) \cdot d(\rho y_1) + (1/(\Gamma_1^{y_1}) + (1/(\Gamma_2^{y_2})) + \cdots + (1/(\Gamma_n^{y_n})) \cdot d(\rho y_2) + \cdots
\]

in that case, the derivative forms of \( 1/\Gamma \) are:

\[
a = y_1 \left( \frac{1}{\Gamma_1} \right)' + y_2 \left( \frac{1}{\Gamma_2} \right)' + \cdots + y_n \left( \frac{1}{\Gamma_n} \right)'
\]

according to the deductions above, the expressions of \( \phi, \varphi \) and \( \psi \) can be obtained:

\[
\phi = y_1 \left( \frac{1}{\Gamma_1} \right)' + y_2 \left( \frac{1}{\Gamma_2} \right)' + \cdots + y_n \left( \frac{1}{\Gamma_n} \right)'
\]

\[
\varphi = y_1 \left( \frac{p_{\text{ref}1}}{\Gamma_1} \right)' + y_2 \left( \frac{p_{\text{ref}2}}{\Gamma_2} \right)' + \cdots + y_n \left( \frac{p_{\text{ref}n}}{\Gamma_n} \right)'
\]

\[
\psi = y_1 (\rho e_{\text{ref}1})' + y_2 (\rho e_{\text{ref}2})' + \cdots + y_n (\rho e_{\text{ref}n})'
\]

The expression forms of mixture rules (8) and (6) are similar. Nevertheless, it must be noticed that:

• In the original rules as (6), the items \( \frac{1}{\Gamma}, \frac{p_{\text{ref}}}{\Gamma} \) and \( \rho e_{\text{ref}} \) are functions of \( \rho \), while in the modified rules as (8), these three items are functions of \( \rho y_i \).

• In the original rules as (6), the volume fraction \( z_i \) is computed by a non-conservative transport equation (4);

while in the modified rules as (8), the mass fraction \( y_i \) is computed conservatively by (5).

3 The Influence of Mixture Rules

3.1 Influence on \( \varphi \) and \( \psi \)

Here we concern these three parameters affected by rules: \( \Gamma, p_{\text{ref}} \) and \( e_{\text{ref}} \). The \( p_{\text{ref}} \) and \( e_{\text{ref}} \) describe the initial reference states, which always depend on the specific volume \( V (V=1/\rho) \). The reference states present the relationship between \( p \) and \( V \), as shown in Figure 1.

Figure 1. Reference states in \( p-V \) relationship.

Here we list some reference states in Mie-Grüneisen EOS. First, the JWL (Jones-Wilkins-Lee) EOS is:

\[
\begin{align*}
\Gamma &= \omega_v, \\
p_{\text{ref}} &= A e^{-\frac{V}{V_0}} + B e^{-\frac{V}{V_0}} \\
e_{\text{ref}} &= \frac{V_0}{R_1} e^{-\frac{V}{V_0}} + \frac{B V_0}{R_2} e^{-\frac{V}{V_0}}
\end{align*}
\]

then the CC(Cochran–Chan) EOS is:

\[
\begin{align*}
\Gamma &= \Gamma_v, \\
p_{\text{ref}} &= A V_0 \left( \frac{V}{V_0} \right)^{-\gamma} - B \left( \frac{V}{V_0} \right)^{-\gamma} \\
e_{\text{ref}} &= \omega_v \left( \frac{V}{V_0} \right)^{-\gamma} - 1 + \frac{B \omega_v}{\rho_v (1-\varepsilon)} \left( \frac{V}{V_0} \right)^{-\gamma} - 1
\end{align*}
\]

and the Mie-Grüneisen of Hugoniot curve:

\[
\begin{align*}
\Gamma &= \Gamma_v \frac{V}{V_0}, \\
p_{\text{ref}} &= p_0 + c_0^2 (V_0 - V) \\
e_{\text{ref}} &= e_0 + \frac{1}{2} (p_{\text{ref}} - p_0) (V_0 - V)
\end{align*}
\]

According to the Figure 1 and EOS (9)(10)(11), it is obvious that the parameter \( p_{\text{ref}} \) increases quickly as the density \( \rho \) becomes larger (\( V \) becomes lower). And the \( \phi \) and \( \psi \) are also increasing functions of \( \rho \). So the \( z_i \) mixture rules, which don’t distinguish \( \rho y_i \) and \( \rho \), would enlarge the values of \( \phi \) and \( \psi \). Comparing with \( \phi \) and \( \psi \), the affection on parameter \( \varphi \) is always very small.
3.2 Influences on Sound Speed

Although the forms of mixture rules play an important role in the calculation, the mixture rules don’t cause any effects on the region beyond the interface. That means the affection of rules only occurs near the interface and the parameters far from the interface are not affected.

At the interface, there’s another important parameter: sound speed $c$. It is defined as:

$$ c^2 = \frac{\partial p}{\partial \rho} + \rho \frac{\partial p}{\partial \rho e} $$

(12)

according to the EOS (2), it is obviously that:

$$ c^2 = \frac{H - \rho u^2}{\Gamma} $$

(13)

where $H = \rho E + p$. For $z_i$ mixture rules, the enlarged $\phi$ and $\psi$ always produce peak values of $c$ at interface. This peak value is not inconsistent with the actual states. However, the peak value is hard to be seen in the normal transition of $c$, in which the fluctuating is usually low. While for the $y_i$ mixture rules, as the component density is taken into account, the peak transition can be avoided.

3.3 Defining of Time Step

The time step has a close relationship to sound speed $c$. To keep the stability in calculation, the time step $\Delta t$ is defined as:

$$ \Delta t = CFL \frac{\Delta x}{\max(|u_j| + c_j)} $$

(14)

the algorithm is stable only when $\text{CFL} \leq 1$. In our calculation, we set a default value of $\text{CFL} = 0.4$ for the examples.

As sound speed $c$ becomes larger, the time interval of the step would become smaller, that means the process of calculation becomes lower.

4 Numerical Scheme

4.1. MUSCL TVD Scheme

For 1-D Cartesian coordinate system, the finite-volume scheme is:

$$ \frac{U_{j+1/2}^{n+1} - U_{j+1/2}^n + F_{j+1/2} - F_{j-1/2}}{\Delta t} = 0 $$

where the bottom corner symbol $j$ denote the $j$th node, the top corner symbol $n$ denotes the time step. $F_{j+1/2}$ is the MUSCL flux:

$$ F_{j+1/2} = \frac{1}{2} \left[ F(U_{j+1/2}^n) + F(U_{j-1/2}^n) - R \left| U_{j+1/2}^n - U_{j-1/2}^n \right| \right] $$

(15)

where the $U_{L,j+1/2}^n$ and $U_{R,j+1/2}^n$ are variables of left and right states at the $j$th grid. $A, L$ and $R$ are the eigenvalues matrix, left and right eigenvector matrices of $\partial \mathbf{F}/\partial \mathbf{U}$. The hat symbol $\wedge$ denotes an average between $j$th and $j+1$th grid. The variables $U_{L,j+1/2}^n$ and $U_{R,j+1/2}^n$ are calculated in a TVD form:

$$ \begin{align*}
U_{L,j+1/2}^n &= U_{j+1/2}^n + \frac{1}{2} R_{j+1/2} W_{L,j} \\
U_{R,j+1/2}^n &= U_{j+1/2}^n - \frac{1}{2} R_{j+1/2} W_{R,j}
\end{align*} $$

where $R_{j+1/2}$ are right eigenvalues matrix at the $j$th node. $W_{L,j}$ and $W_{R,j}$ are column vectors, in which the elements are $w_{L,j}$ and $w_{R,j}$, respectively. The expressions of $w_{L,j}$ and $w_{R,j}$ are:

$$ \begin{align*}
w_{L,j} &= D_{j}^n \left( 1 - \lambda_{j+1/2} \frac{\Delta t}{\Delta x} \right) \\
w_{R,j} &= D_{j}^n \left( 1 + \lambda_{j+1/2} \frac{\Delta t}{\Delta x} \right)
\end{align*} $$

in which $\lambda_{j+1/2}$ are left eigenvalues matrix at the $j$th node. And the matrix $D_{j+1/2}^n$ is:

$$ D_{j}^n = \min \left[ L_{j+1/2}(U_{j+1} - U_j), L_{j+1/2}(U_j - U_{j+1}) \right] $$

4.2. Roe Solver

$$ F_{j+1/2} = \frac{1}{2} \left[ F(U_{L,j+1/2}^n) + F(U_{R,j+1/2}^n) - 2 R \left| U_{j+1/2}^n - U_{j-1/2}^n \right| \right] $$

(15), there are many average forms of $\wedge$. Here we use a popular Roe average form [12], which are:

$$ \begin{align*}
\hat{\rho} &= \sqrt{\rho_L \rho_R} + \sqrt{\rho_L \rho_R} \\
\hat{u} &= \frac{\rho_L u_L + \rho_R u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}} \\
\hat{H} &= \frac{\rho_L H_L + \rho_R H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}
\end{align*} $$

for $\Gamma$ and $p$, we use similar form as Shyue[4]:

$$ \frac{1}{\Gamma} = \frac{1}{\sqrt{\rho_L} + \sqrt{\rho_R}} \left( \sqrt{\rho_L} / \Gamma_L + \sqrt{\rho_R} / \Gamma_R \right) $$

$$ \frac{\hat{p}}{\Gamma} = \frac{1}{\sqrt{\rho_L} + \sqrt{\rho_R}} \left( \rho_L \sqrt{\rho_L} / \Gamma_L + \rho_R \sqrt{\rho_R} / \Gamma_R \right) $$

then the sound speed $c$ can be written as:

$$ \hat{c} = \sqrt{\hat{H} - \hat{u}^2 - \hat{\rho} \phi - \psi} $$
as the \( \phi \), \( \varphi \) and \( \psi \) represent the values at the node, so there is no need to consider the average for these three items.

### 5 Examples

#### 5.1. Gaseous Explosive-copper Problem

The first mixture problem is an interaction problem of gaseous explosive-copper. The problem is investigated by Saurel and Abgrall[6]. Initially, gaseous explosive and solid copper are placed at the left and right sides, respectively. The explosive is modeled by JWL EOS as (9). The other component copper is modeled by C-C EOS as (10). The coefficients for these two EOSs are:

- **Explosive (JWL):** \( \rho_0 = 1840 \text{kg/m}^3 \), \( \Gamma_0 = 0.25 \), \( A = 845.5 \text{Gpa} \), \( B = 20.5 \text{Gpa} \), \( R_1 = 4.6 \), \( R_2 = 1.35 \)
- **Copper (CC):** \( \rho_0 = 8900 \text{kg/m}^3 \), \( \Gamma_0 = 2 \), \( A = 145.67 \text{Gpa} \), \( B = 147.75 \text{Gpa} \), \( \varepsilon_1 = 2.99 \), \( \varepsilon_2 = 1.99 \)

![Figure 2. Solution of Gaseous Explosive-copper problem.](image)

In order to test the performances of the original and modified rules, results of the \( \rho \) and \( p \) are given in Figure 2. It is found that both the two solutions are near the same. The main difference for the two mixture rules are steps cost in calculation. For modified rules about \( y_i \), the steps reduce nearly 10%.

The steps difference results from transition form at interface. As the mixture rules are different, transition forms are also different. The mixture rules of \( z_i \) obtain high values of \( \phi \) and \( \psi \), as shown in Figure 3. In comparison, the mixture rules of \( y_i \) get the low values of \( \phi \) and \( \psi \) at the interface. According to Figure 1, the pressure decreases quickly as \( V \) increases. That means the peak value of \( z_i \) mixture rules is not theoretically correct.

![Figure 3. Curves of \( \phi \) and \( \psi \) for Different Mixtures Rules.](image)

The transition of \( \phi \) and \( \psi \) then affects the sound speed \( c \), as shown in Figure 4. It is found that the curve of original mixture rules fluctuates so much. According to (14), it is clearly that the peak value of \( c \) decreases the time interval and brings more steps in calculation.

![Figure 4. Curves of \( c \) in Gaseous Explosive-copper problem.](image)
5.2. Solid Explosive-copper Problem

This is another two-component shock tube problem of Saurel and Abgrall[6]. The explosive is in a solid state initially, and goes rightwards with a high speed. Both the solid explosive and copper are modelled by JWL EOS, with the relative coefficients as:

- Copper(CC): \( \rho_0=8900 \text{kg/m}^3 \), \( \Gamma_0=2.00 \), \( A=145.67 \text{Gpa} \), \( B=147.75 \text{Gpa} \), \( \epsilon_1=2.99 \), \( \epsilon_2=1.99 \)

- Explosive(CC): \( \rho_0=1840 \text{kg/m}^3 \), \( \Gamma_0=0.93 \), \( A=12.87 \text{Gpa} \), \( B=13.42 \text{Gpa} \), \( \epsilon_1=4.1 \), \( \epsilon_2=3.1 \)

Figure 5 gives the solutions of original and modified rules. The two solutions are both very close to the exact solution. But the modified mixture rules cost much less steps than original rules.

Then our attentions are transferred to the sound speed \( c \). Figure 6 are the \( c \) curve of these two rules. It can be seen that the two solutions are quite different near the interface. The original mixture rules produce a great peak in the curves.

| Grids | Original Rules | Modified Rules |
|-------|----------------|----------------|
| 100   | 416 steps      | 118 steps      |
| 200   | 849 steps      | 234 steps      |
| 300   | 1295 steps     | 357 steps      |

Table 1. Amount of Steps in Different Grids System.

5.3. Classical Underwater explosion Problem

A classical experiment about underwater free explosion, which investigated by Cole [[13]], is considered here. The TNT charge is placed in water and modelled by JWL EOS (9), with the coefficients as:

- Explosive (JWL): \( \rho_0=1630 \text{kg/m}^3 \), \( \Gamma_0=0.3 \), \( A=371.2 \text{Gpa} \), \( B=3.21 \text{Gpa} \), \( R_1=4.15 \), \( R_2=0.95 \)

the other component water is modelled by a piecewise Mie-Grüneisen EOS:

\[
\Gamma = \gamma_0 + \alpha \mu \\
\rho_\text{ref} = \begin{cases} 
\rho_0 \frac{\mu (1+\mu)}{1-(s_1-1)\mu - \frac{\mu^2}{\mu+1} - s_2 \frac{\mu^2}{(\mu+1)^2}} & (\rho \geq \rho_0) \\
\rho_0 \frac{\mu}{\mu+1} & (\rho < \rho_0) 
\end{cases} \\
e_\text{ref} = \begin{cases} 
\frac{c_0^2 \mu^2}{2} & (\rho \geq \rho_0) \\
0 & (\rho < \rho_0)
\end{cases}
\]

the EOS of water includes the compressed and expanded states. As the explosive charge explodes, the gaseous product interacts with water and produce shock waves.

Figure 7. Pressure Distribution of the two rules.
Here the travelling of shock wave is simulated by the two mixture rules, and the pressure distributions are shown in Figure 7, in which $R_0$ is the radius of the charge. Unlike the former two examples, the results are not the same for two rules. The difference is caused by the spherical coordinate system. In the spherical system, the pressure reduces as the distance increases. However, the property isn’t taken into account in the original mixture rules, so the pressure becomes higher than actual value.

To test the accuracy, the pressure-time evolutions of two rules are compared with empirical data, the results are shown in Figure 8. It is obvious that the modified mixture rules can get more accurate pressure. The peak values in original rules are more closed to the empirical values.

Then we concern the sound speed $c$, which is shown in Figure 9. The curves of $c$ in original mixture rules are also abnormally high. The peak value, which resulted by the original rules, makes the calculation much longer.

In Table 2, it can be watched that the original rules need more steps then the modified mixture rules. So the modified rules are more effective in calculation.

### Conclusion

Our main attentions are focused on the modification of the mixture rules in Mie-Grüneisen mixture model. The original mixture rules, which produce irregular curve of sound speed at the interface, affect the time step in calculation. In comparison to the original mixture rules, the modified rules limit the violent changes of sound speed and improve the efficiency of the calculation. Numerical examples show that the modified rules can reduce time step obviously. In the addition, the modified rules can get more accurate solution in spherical system.

| Location of the shock wave | Original Rules | Modified Rules |
|----------------------------|----------------|----------------|
| Reach 5 $R_0$              | 2178 steps     | 1560 steps     |
| Reach 10 $R_0$             | 5770 steps     | 4020 steps     |
| Reach 15 $R_0$             | 9771 steps     | 6807 steps     |
| Reach 20 $R_0$             | 13940 steps    | 9861 steps     |

Figure 8. The $p$-$t$ curves at different positions.

Figure 9. Curves of $c$ in underwater explosion problem.
Acknowledgements

The research work is funded by National Natural Science Foundation of China (Project Number: A17292) and Guangdong Natural Science Foundation (Grant Number: 2017A030313275), as well as Higher Education of Guangdong (Foundation for Distinguished Young Talents, Project Number: Q17109/2017052623).

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