

Modified Baer-Nunziato Model for the Simulation of Interfaces Between Compressible Fluids

Qiang Wu^{1,†}, Xian-Guo Lu² and De-Kang Mao^{1,*}

¹ Department of Mathematics, Shanghai University, Shanghai 200444, China.

² Accounting Institute, Shanghai Institute of Foreign Trade, Wenxiang Road 1900, Songjiang, Shanghai, China.

Received 2 August 2009; Accepted (in revised version) 13 September 2010

Available online 10 November 2010

Abstract. In this paper we proposed a modified Baer-Nunziato model for compressible multi-fluid flows, with main attention on the energy exchange between the two fluids. The proposed model consists of eleven PDEs; however, the use of the particular phase evolving variables may reduce the model to have only six PDEs. The main advantage of the model is that the Abgrall's UPV criterion on mixture velocity and pressure is satisfied without affecting either its hyperbolicity or its conservations of the two individual masses, momentum or total energy. An Lax-Friedrichs scheme is built for a particular case of the proposed model. When the two fluids in the fluid mixture are both of the linear Mie-Gruneisen type, the scheme satisfies the Abgrall's UPV criterion on mixture velocity and pressure. Numerical experiments with polytropic, barotropic, stiffened and van der Waals fluids show that the scheme is efficient and able to treat fluids characterized with quite different thermodynamics.

AMS subject classifications: 65M06, 35L65, 76N15, 76M10

Key words: Baer-Nunziato model, hyperbolicity, Abgrall's UPV criterion.

1 Introduction

The Baer-Nunziato (BN) model, see [2–5] and [8], is a two-mass, two-velocity and two-pressure diffuse model for multi-fluid flows. The model, by omitting the mass transfer, drag force, chemical reaction and convective heat exchange, has the form

$$\frac{\partial \alpha_1 \hat{\rho}_1}{\partial t} + \frac{\partial \alpha_1 \hat{\rho}_1 u_1}{\partial x} = 0, \quad (1.1a)$$

$$\frac{\partial \alpha_1 \hat{\rho}_1 u_1}{\partial t} + \frac{\partial (\alpha_1 \hat{\rho}_1 u_1^2 + \alpha_1 \hat{p}_1)}{\partial x} = p \frac{\partial \alpha_1}{\partial x}, \quad (1.1b)$$

[†]Current address: Mathematics College, Hefei University of Technology, Hefei 230009, China.

*Corresponding author. *Email addresses:* wqwq11@sohu.com (Q. Wu), luxianguo403@163.com (X.-G. Lu), dkmao@staff.shu.edu.cn (D.-K. Mao)

$$\frac{\partial \alpha_1 \hat{\rho}_1 E_1}{\partial t} + \frac{\partial u_1 (\alpha_1 \hat{\rho}_1 E_1 + \alpha_1 \hat{p}_1)}{\partial x} = p u \frac{\partial \alpha_1}{\partial x}, \quad (1.1c)$$

$$\frac{\partial \alpha_2 \hat{\rho}_2}{\partial t} + \frac{\partial \alpha_2 \hat{\rho}_2 u_2}{\partial x} = 0, \quad (1.1d)$$

$$\frac{\partial \alpha_2 \hat{\rho}_2 u_2}{\partial t} + \frac{\partial (\alpha_2 \hat{\rho}_2 u_2^2 + \alpha_2 \hat{p}_2)}{\partial x} = p \frac{\partial \alpha_2}{\partial x}, \quad (1.1e)$$

$$\frac{\partial \alpha_2 \hat{\rho}_2 E_2}{\partial t} + \frac{\partial u_2 (\alpha_2 \hat{\rho}_2 E_2 + \alpha_2 \hat{p}_2)}{\partial x} = p u \frac{\partial \alpha_2}{\partial x}, \quad (1.1f)$$

$$\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} = 0, \quad (1.1g)$$

where $\hat{\rho}_k$ is the phase density, u_k is the phase velocity, \hat{p}_k is the phase pressure, $E_k = u_k^2/2 + \epsilon_k$ is the specific phase total energy of the k th fluid with ϵ_k the specific phase internal energy, α_k is the volume fraction satisfying the saturation condition

$$\alpha_1 + \alpha_2 = 1, \quad (1.2)$$

and finally, u and p are the averaged interfacial velocity and pressure. There are different ways to compute the interfacial velocity and pressure corresponding to different physics, e.g., in [8] they are computed as the mixture velocity,

$$u = \frac{\alpha_1 \hat{\rho}_1 u_1 + \alpha_2 \hat{\rho}_2 u_2}{\alpha_1 \hat{\rho}_1 + \alpha_2 \hat{\rho}_2}, \quad (1.3)$$

and mixture pressure,

$$p = p_1 + p_2 = \alpha_1 \hat{p}_1 + \alpha_2 \hat{p}_2, \quad (1.4)$$

respectively, where

$$\hat{p}_k = P_k(\hat{\rho}_k, \epsilon_k) \quad (1.5)$$

is the phase pressure computed by the EOS of the k th fluid as in Eq. (2.1) and $p_k = \alpha_k \hat{p}_k$ is the partial pressure contributed by the k th fluid.

The system is not conservative, and the source terms in the momentum and energy equations, called nozzling terms [3], correspond to the momentum and energy exchange between the two fluids. Although the model is complex, it is unconditionally hyperbolic and is able to treat fluids characterized by very different thermodynamics because each fluid uses its own EOS.

The Abgrall's uniform-pressure-velocity (UPV) criterion requires that a two-phase flow, uniform in pressure and velocity, must remain uniform on the same variables during its temporal evolution (see [8,9]). The BN model (1.1) and its numerical methods can meet the Abgrall's UPV criterion by requiring

$$u_1 = u_2 = \text{const}, \quad \hat{p}_1 = \hat{p}_2 = \text{const}; \quad (1.6)$$

i.e., the two fluids are in velocity and pressure equilibriums with each other [8]. However, directly assuming pressure equilibrium will result in the loss of hyperbolicity of the model. In practice, relaxations that drive the fluids towards the velocity and pressure equilibriums are added to the BN model in numerical simulations, see, e.g., [4,6,8], which surely adds complexities.

In this paper we propose a modified BN model. The work is a further extension of [14]. The modification is mainly on the energy exchange between the two fluids in the work done by the pressure. The modified model meets the Abgrall's UPV criterion by requiring only the velocity equilibrium, and in this way the hyperbolicity of the model is not affected. An Lax-Freidrichs (LxF) scheme for a particular case of the model is constructed and is proved to meet the UPV criterion on mixture velocity and pressure for linear Mie-Gruneisen fluids. Numerical experiments on Riemann problems with a wide range of different fluids show that the scheme is efficient. Second-order extension of the LxF scheme has been obtained in the way of [7] and the numerical experiments showed great improvement over the first-order schemes. However, the extension is not straightforward and will be reported in another work. Nevertheless, a numerical example will be presented to show the improvement of the second-order extension over the first-order schemes.

The rest of the paper is organized in the following fashion. In Section 2 we present the modified BN model and discuss its properties, especially those relevant to the UPV criterion. In Section 3 we present the LxF scheme for the particular case of the modified model. Section 4 presents the numerical tests performed with the LxF scheme. Finally, we conclude the paper in Section 5.

2 The modified BN model

Assume that the EOS's of the two fluids in the fluid mixture are

$$p = P_k(\rho, \epsilon), \quad k = 1, 2, \quad (2.1)$$

respectively. According to the thermodynamics,

$$(P_k)_\rho > 0 \quad \text{and} \quad (P_k)_\epsilon > 0. \quad (2.2)$$

We assume that the EOS of each fluid can be decomposed as

$$P_k(\rho, \epsilon) = P_{k,1}(\rho, \epsilon) + P_{k,2}(\rho, \epsilon), \quad (2.3)$$

with

$$(P_{k,l})_\rho \geq 0 \quad \text{and} \quad (P_{k,l})_\epsilon \geq 0, \quad l = 1, 2. \quad (2.4)$$

Note that the original EOS of the fluid can be recovered by setting $P_{k,1}(\rho, \epsilon) = P_k(\rho, \epsilon)$ and $P_{k,2}(\rho, \epsilon) \equiv 0$. As a result, the assumption Eqs. (2.3) and (2.4) adds no restriction on the EOS's.

We assume velocity equilibrium in our modified BN model, i.e., $u_1 = u_2 = u$. The model that describes the balance laws of masses, momentum and energies of the two fluids is then governed by

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 u}{\partial x} = 0, \quad (2.5a)$$

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 u}{\partial x} = 0, \quad (2.5b)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0, \quad (2.5c)$$

$$\frac{\partial \rho_1 E_1}{\partial t} + \frac{\partial u \rho_1 E_1}{\partial x} + \frac{\rho_1}{\rho} \frac{\partial u p}{\partial x} = 0, \quad (2.5d)$$

$$\frac{\partial \rho_1 E_2}{\partial t} + \frac{\partial u \rho_1 E_2}{\partial x} + \frac{\rho_2}{\rho} \frac{\partial u p}{\partial x} = 0, \quad (2.5e)$$

where $\rho_k = \alpha_k \hat{\rho}_k$ is the partial density of the k th fluid, $\rho = \rho_1 + \rho_2$ is the mixture density and p is the mixture pressure. To close the model, we need to provide a way to compute the mixture pressure. To this end, we introduce four sets of nonnegative phase evolving variables, $(\alpha_{1,l}, \alpha_{2,l})$ and $(\beta_{1,l}, \beta_{2,l})$, $l = 1, 2$, each of which satisfies the phase advection equation

$$\frac{\partial \chi_{k,l}}{\partial t} + u \frac{\partial \chi_{k,l}}{\partial x} = 0, \quad (2.6)$$

with $\chi = \alpha$ or β . The $\alpha_{k,l}$'s satisfy the saturation conditions

$$\alpha_{1,l} + \alpha_{2,l} = 1, \quad l = 1, 2. \quad (2.7)$$

Also $\alpha_{1,l} = 1$ ($\alpha_{2,l} = 0$) and $\beta_{1,l} = 1$ in the first fluid and $\alpha_{1,l} = 0$ ($\alpha_{2,l} = 1$) and $\beta_{2,l} = 1$ in the second fluid for $l = 1, 2$. Then the mixture pressure is computed as

$$p = p_1 + p_2, \quad (2.8)$$

where the two partial pressures are computed as

$$p_1 = \alpha_{1,1} P_{1,1}(\beta_{1,1} \rho_1, \epsilon_1) + \alpha_{1,2} P_{1,2}(\beta_{1,2} \rho_1, \epsilon_1), \quad (2.9a)$$

$$p_2 = \alpha_{2,1} P_{2,1}(\beta_{2,1} \rho_2, \epsilon_2) + \alpha_{2,2} P_{2,2}(\beta_{2,2} \rho_2, \epsilon_2), \quad (2.9b)$$

with the two EOS's having decompositions (2.3)-(2.4). Thus, we complete the modified model, which is a system of eleven PDEs.

Remark 2.1. It is easy to see that the two mass equations in the modified model, (2.5a) and (2.5b), are just the same as (1.1a) and (1.1d) in the original model, and the momentum equation in the modified model, (2.5c), is just the sum of the two momentum equations

(1.1b) and (1.1e) in the original model. Therefore, the major difference between the original and modified BN models lies in the two balance laws of energy. If we write (2.5d) and (2.5e) as

$$\frac{\partial \rho_1 E_1}{\partial t} + \frac{\partial u(\rho_1 E_1 + \frac{\rho_1}{\rho} p)}{\partial x} = pu \frac{\partial \frac{\rho_1}{\rho}}{\partial x}, \tag{2.10a}$$

$$\frac{\partial \rho_2 E_1}{\partial t} + \frac{\partial u(\rho_1 E_2 + \frac{\rho_2}{\rho} p)}{\partial x} = pu \frac{\partial \frac{\rho_2}{\rho}}{\partial x}, \tag{2.10b}$$

and compare them with (1.1c) and (1.1f), we see that the modification corresponds to replacing the volume fractions and phase pressures with the mass fractions and mixture pressures, respectively, in the original BN model.

Remark 2.2. The introduction of $\alpha_{k,l}$'s and $\beta_{k,l}$'s provides freedom to describe the thermodynamics of the fluid mixture rather than imposes restriction on it, and particular choices of them may reduce the dimension of system (2.5). For example, we can set the decomposition (2.3)-(2.4) as

$$P_{k,1}(\rho, \epsilon) = P_k(\rho, \epsilon), \quad \text{and} \quad P_{k,2}(\rho, \epsilon) \equiv 0, \tag{2.11}$$

set $\alpha_{1,1} = \alpha_1$, $\alpha_{2,1} = \alpha_2$, $\beta_{1,1} = 1/\alpha_1$ and $\beta_{2,1} = 1/\alpha_2$, where α_1 and α_2 are the two volume fractions, and abandon $\alpha_{1,2}$, $\beta_{1,2}$, $\alpha_{2,2}$ and $\beta_{2,2}$. Then (2.8)-(2.9) recovers mixture pressure computation (1.4) and (1.5), and in this case, the system is reduced to consist of only six PDEs.

Theorem 2.1. *The proposed model (2.5) has the following properties:*

- (1) it recovers the standard Euler system when only one fluid is present;
- (2) it conserves the masses of individual fluids as well as of the fluid mixture, the mixture momentum and the mixture total energy;
- (3) it is unconditionally hyperbolic.

Proof. The first two conclusions of the theorem are obvious, and we thus only prove the third one. To this end, we write the system (2.5) in the primitive variables

$$\frac{\partial w}{\partial t} + A(w) \frac{\partial w}{\partial x} = 0, \tag{2.12}$$

where

$$w = (\rho_1, \rho_2, u, p_1, p_2, \alpha_{1,1}, \alpha_{1,2}, \beta_{1,1}, \beta_{1,2}, \beta_{2,1}, \beta_{2,2})^T.$$

By calculation we can obtain from (2.5) that

$$\frac{\partial \rho_1}{\partial t} + u \frac{\partial \rho_1}{\partial x} + \rho_1 \frac{\partial u}{\partial x} = 0, \tag{2.13a}$$

$$\frac{\partial \rho_2}{\partial t} + u \frac{\partial \rho_2}{\partial x} + \rho_2 \frac{\partial u}{\partial x} = 0, \tag{2.13b}$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \left(\frac{\partial p_1}{\partial x} + \frac{\partial p_2}{\partial x} \right) = 0, \tag{2.13c}$$

$$\frac{\partial p_1}{\partial t} + u \frac{\partial p_1}{\partial x} + \kappa_1 \frac{\partial u}{\partial x} = 0, \tag{2.13d}$$

$$\frac{\partial p_2}{\partial t} + u \frac{\partial p_2}{\partial x} + \kappa_2 \frac{\partial u}{\partial x} = 0, \tag{2.13e}$$

where

$$\kappa_1 = \sum_{l=1}^2 \left\{ \alpha_{1,l} \beta_{1,l} (P_{1,l})_{\rho} \rho_1 + \alpha_{1,l} \frac{(P_{1,l})_{\epsilon} p}{\rho} \right\}, \tag{2.14a}$$

$$\kappa_2 = \sum_{l=1}^2 \left\{ \alpha_{2,l} \beta_{2,l} (P_{2,l})_{\rho} \rho_2 + \alpha_{2,l} \frac{(P_{2,l})_{\epsilon} p}{\rho} \right\}. \tag{2.14b}$$

By taking the six independent PDEs in (2.6) as we obtain the coefficient matrix $A(w)$ in (2.13),

$$A(w) = \begin{bmatrix} u & 0 & \rho_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & u & \rho_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & u & \frac{1}{\rho} & \frac{1}{\rho} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \kappa_1 & u & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \kappa_2 & 0 & u & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & u & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & u & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & u & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & u \end{bmatrix}. \tag{2.15}$$

It is easy to obtain the eigenvalues of $A(w)$,

$$\lambda_1 = u - c, \quad \lambda_{2,3,4,5,7,8,9,10} = u, \quad \lambda_{11} = u + c, \tag{2.16}$$

with the sound speed

$$c = \sqrt{\frac{\kappa_1 + \kappa_2}{\rho}}. \tag{2.17}$$

The positivity of $\rho_1, \rho_2, p, \alpha_{k,l}$'s, $\alpha_{k,l}$'s together with (2.4) guarantees the reality of c , from which the hyperbolicity of the model follows. \square

Theorem 2.2. *If initially the fluid has uniform velocity and mixture pressure, then the modified model maintains the velocity and mixture pressure to be uniform during the temporal evolution.*

Proof. Assume that the velocity and mixture pressure are initially constant u_0 and p_0 , respectively. Firstly, we obtain the velocity evolution equation from (2.13c),

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0. \quad (2.18)$$

Secondly, by summing up (2.13d) and (2.13e), we obtain the mixture pressure evolution equation

$$\frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + (\kappa_1 + \kappa_2) \frac{\partial u}{\partial x} = 0. \quad (2.19)$$

It is obvious that $u(x,t) = u_0$ and $p(x,t) = p_0$ are the unique solution to (2.18) and (2.19) that satisfies the initial conditions $u(x,0) = u_0$ and $p(x,0) = p_0$. The proof is thus completed. \square

We conclude this section by considering an example of the modified BN model. We know that nearly all fluids are of the Mie-Gruneisen type

$$P(\rho, \epsilon) = (\gamma - 1)(\rho\epsilon + \mathcal{A}\rho) - \gamma\mathcal{B}, \quad (2.20)$$

with $\gamma > 1$, $\mathcal{A} > 0$ and $\mathcal{B} > 0$. We call EOS (2.20) of linear Mie-Gruneisen type when all γ , \mathcal{A} and \mathcal{B} are constant. The linear Mie-Grunesien type of fluids include

$$\text{polytropic:} \quad p = (\gamma - 1)\rho\epsilon, \quad (2.21a)$$

$$\text{barotropic:} \quad p = (\gamma - 1)\left(\rho\epsilon + \frac{\mathcal{B}\rho}{\rho_0}\right) - \gamma\mathcal{B}, \quad (2.21b)$$

$$\text{stiffened:} \quad p = (\gamma - 1)\rho\epsilon - \gamma\mathcal{B}. \quad (2.21c)$$

If both the fluids are of the linear Mie-Gruneisen type but with different coefficients, we decompose each EOS as

$$P_{k,1}(\rho, \epsilon) = (\gamma_k - 1)(\rho\epsilon + \mathcal{A}_k\rho), \quad P_{k,2}(\rho, \epsilon) = -\gamma_k\mathcal{B}_k, \quad k = 1, 2. \quad (2.22)$$

It is easy to verify that (2.4) holds for this decomposition. Now we choose $(\alpha_{1,1}, \alpha_{2,1})$ to be the mass fractions $(\rho_1/\rho, \rho_2/\rho)$, which satisfy the phase advection equation (2.6); choose $(\alpha_{1,2}, \alpha_{2,2})$ to be the two volume fractions, (α_1, α_2) ; choose $\beta_{1,1} \equiv 1$ and $\beta_{2,1} \equiv 1$, and abandon $\beta_{1,2}$ and $\beta_{2,2}$. With this setting, the two partial pressures become

$$p_k = (\gamma_k - 1)(\rho_k\epsilon_k + \mathcal{A}_k\rho_k) - \alpha_k\gamma_k\mathcal{B}_k, \quad k = 1, 2, \quad (2.23)$$

and the system (2.5) is reduced to have six PDEs. It is easy to obtain the two κ 's in (2.14),

$$\kappa_k = \frac{\rho_k}{\rho} \left(p_k + \alpha_k(\gamma_k\mathcal{B}_k + (\gamma_k - 1)p) \right), \quad k = 1, 2. \quad (2.24)$$

Note that the sound speed c then computed by (2.17) is different from that of the reduced BN model with velocity equilibrium in [3]; the latter is simply the mass average of the two sound speeds.

3 The Lax-Friedrichs scheme

In this section we proposed a Lax-Friedrich (LxF) scheme for the modified BN model of the linear Mie-Gruneisen type. The phase evolving variables are chosen as those given in the end of the previous section, and thus the model is reduced to six PDEs. The LxF scheme, which uses stagger grids, is then given by:

$$\bar{\rho}_{1,i+\frac{1}{2}} = \frac{1}{2}(\rho_{1,i} + \rho_{1,i+1}) - \frac{\lambda}{2}(\rho_{1,i+1}u_{i+1} - \rho_{1,i}u_i), \tag{3.1a}$$

$$\bar{\rho}_{2,i+\frac{1}{2}} = \frac{1}{2}(\rho_{2,i} + \rho_{2,i+1}) - \frac{\lambda}{2}(\rho_{2,i+1}u_{i+1} - \rho_{2,i}u_i), \tag{3.1b}$$

$$\bar{\rho}_{i+\frac{1}{2}}\bar{u}_{i+\frac{1}{2}} = \frac{1}{2}(\rho_i u_i + \rho_{i+1} u_{i+1}) - \frac{\lambda}{2}(\rho_{i+1} u_{i+1}^2 + p_{i+1} - \rho_i u_i^2 - p_i), \tag{3.1c}$$

$$\begin{aligned} \bar{\rho}_{1,i+\frac{1}{2}}\bar{E}_{1,i+\frac{1}{2}} &= \frac{1}{2}(\rho_{1,i}E_{1,i} + \rho_{1,i+1}E_{1,i+1}) - \frac{\lambda}{2}(\rho_{1,i+1}E_{1,i+1}u_{i+1} - \rho_{1,i}E_{1,i}u_i) \\ &\quad - \frac{\lambda}{2} \frac{\rho_{1,i} + \rho_{1,i+1}}{\rho_i + \rho_{i+1}}(u_{i+1}p_{i+1} - u_i p_i), \end{aligned} \tag{3.1d}$$

$$\begin{aligned} \bar{\rho}_{2,i+\frac{1}{2}}\bar{E}_{2,i+\frac{1}{2}} &= \frac{1}{2}(\rho_{2,i}E_{2,i} + \rho_{2,i+1}E_{2,i+1}) - \frac{\lambda}{2}(\rho_{2,i+1}E_{2,i+1}u_{i+1} - \rho_{2,i}E_{2,i}u_i) \\ &\quad - \frac{\lambda}{2} \frac{\rho_{2,i} + \rho_{2,i+1}}{\rho_i + \rho_{i+1}}(u_{i+1}p_{i+1} - u_i p_i), \end{aligned} \tag{3.1e}$$

$$\bar{\alpha}_{1,i+\frac{1}{2}} = \frac{1}{2}(\alpha_{1,i} + \alpha_{1,i+1}) - \frac{\lambda}{2} \frac{(u_i + u_{i+1})}{2}(\alpha_{1,i+1} - \alpha_{1,i}), \tag{3.1f}$$

where the quantities with overhead bars are on the next time level and the quantities without overhead bars are on the current time level. The numerical mixture pressure is then computed by

$$p_i = p_{1,i} + p_{2,i}, \tag{3.2}$$

where $p_{k,i}$ is computed as

$$p_{k,i} = (\gamma_k - 1)(\rho_{k,i}\epsilon_{k,i} + \mathcal{A}_k \rho_{k,i}) - \alpha_{k,i} \gamma_k \mathcal{B}_k, \quad k = 1, 2. \tag{3.3}$$

The mesh ratio $\lambda = \tau/h$ with τ and h the spatial and temporal increments is restricted by the CFL condition, i.e., $(|u| + c)\lambda < 1$.

Theorem 3.1. *The proposed scheme (3.1) has the following properties:*

- (1) *it conserves the individual as well as the mixture masses, mixture momentum and energy;*
- (2) *when the CFL condition is satisfied, it maintains the individual masses nonnegative;*
- (3) *it recovers the standard LxF scheme when only one fluid is present.*

Proof. Conclusions (1) and (3) are obvious. To prove (2), we rewrite (3.1a) and (3.1b) as

$$\bar{\rho}_{k,i+\frac{1}{2}} = \frac{1}{2}(1 + \lambda u_i)\rho_{k,i} + \frac{1}{2}(1 - \lambda u_{i+1})\rho_{k,i+1}, \quad k = 1, 2. \tag{3.4}$$

The relevant CFL condition guarantees

$$\lambda \max_i |u_i| < 1, \tag{3.5}$$

and thus yields the nonnegativity of the two coefficients in (3.4). The nonnegativity of the two masses then follows, and thus the proof is complete. \square

Theorem 3.2. *If initially the velocity and mixture pressure are uniform, then the scheme maintains the property that the velocity and mixture pressure are uniform in the computations.*

Proof. According to the UPV assumption of the flow, the numerical solution in the i th cell at t_n is

$$U_i = (\rho_{1,i}, \rho_{2,i}, \rho_i u_0, \rho_{1,i} E_{1,i}, \rho_{2,i} E_{2,i}, \alpha_{1,i}), \tag{3.6}$$

with mixture pressure p_0 , where both u_0 and p_0 are constant. The same situation holds in the $(i+1)$ th cell. According to (3.1h), the two partial pressures in the i th and $(i+1)$ th cells are computed as

$$p_{k,i} = (\gamma_k - 1)(\rho_{k,i} \epsilon_{k,i} + \mathcal{A}_k \rho_{k,i}) - \alpha_{k,i} \gamma_k \mathcal{B}_k, \quad k=1,2, \tag{3.7a}$$

$$p_{k,i+1} = (\gamma_k - 1)(\rho_{k,i+1} \epsilon_{k,i+1} + \mathcal{A}_k \rho_{k,i+1}) - \alpha_{k,i+1} \gamma_k \mathcal{B}_k, \quad k=1,2. \tag{3.7b}$$

To prove the theorem, we need to show that the numerical solution at t_{n+1} is still with the velocity u_0 and mixture pressure p_0 .

Firstly, we have from (3.1a) and (3.1b)

$$\bar{\rho}_{k,i+\frac{1}{2}} = \frac{1}{2}(1 + \lambda u_0) \rho_{k,i} + \frac{1}{2}(1 - \lambda u_0) \rho_{k,i+1}, \quad k=1,2. \tag{3.8}$$

By noting $p_i = p_{i+1} = p_0$, we have from (3.1c)

$$\bar{\rho}_{i+\frac{1}{2}} \bar{u}_{i+\frac{1}{2}} = \frac{1}{2}(1 + \lambda u_0) \rho_i u_0 + \frac{1}{2}(1 - \lambda u_0) \rho_{i+1} u_0, \tag{3.9}$$

which, by noting $\rho_1 + \rho_2 = \rho$, leads to the first conclusion

$$\bar{u}_{i+\frac{1}{2}} = u_0. \tag{3.10}$$

Secondly, by noting the definition of internal energy, (3.8), (3.10) and the uniform mixture pressure p_0 at the current time level, we obtain from (3.1d) and (3.1e)

$$\bar{\rho}_{k,i+\frac{1}{2}} \bar{\epsilon}_{k,i+\frac{1}{2}} = \frac{1}{2}(1 + \lambda u_0) \rho_{k,i} \epsilon_{k,i} + \frac{1}{2}(1 - \lambda u_0) \rho_{k,i+1} \epsilon_{k,i+1}, \quad k=1,2. \tag{3.11}$$

Also using (3.1f) and the saturation condition on α_1 and α_2 gives

$$\bar{\alpha}_{k,i+\frac{1}{2}} = \frac{1}{2}(1 + \lambda u_0) \alpha_{k,i} + \frac{1}{2}(1 - \lambda u_0) \alpha_{k,i+1}, \quad k=1,2. \tag{3.12}$$

We note from (3.8), (3.11) and (3.12) that the evolutions of ρ_k , $\rho_k \epsilon_k$ and α_k , $k=1,2$, are all in the form

$$\bar{\Psi}_{i+\frac{1}{2}} = \frac{1}{2}(1+\lambda u_0)\Psi_i + \frac{1}{2}(1-\lambda u_0)\Psi_{i+1}, \tag{3.13}$$

with $\Psi = \rho_k$, $\rho_k \epsilon_k$ or α_k . We also note from (3.3) that the two partial pressures are all linear combinations of ρ_k , $\rho_k \epsilon_k$ and α_k in the two cells. This leads to

$$\bar{p}_{k,i+\frac{1}{2}} = \frac{1}{2}(1+\lambda u_0)p_{k,i} + \frac{1}{2}(1-\lambda u_0)p_{k,i+1}, \tag{3.14}$$

the evolutions of the two partial pressures are also in the form of (3.13).

Finally, by adding up (3.14) for $k=1,2$ and noting (3.2) in the i th and $(i+1)$ th cells, we have for the mixture pressure

$$\bar{p}_{i+\frac{1}{2}} = \frac{1}{2}(1+\lambda u_0)p_i + \frac{1}{2}(1-\lambda u_0)p_{i+1}. \tag{3.15}$$

The second conclusion then follows from $p_i = p_{i+1} = p_0$, and the proof is thus complete. \square

4 Numerical experiments

In this section, we present a number of numerical tests using the LxF scheme proposed in the previous section. All the tests are Riemann problems of two-fluid flows involving polytropic, barotropic, stiffened and van der Waals gases. The examples are chosen from literatures on interface modeling, and are believed to be widely used to test the efficiency of multi-fluid models and their numerical methods. Brief description of each example will be given, and its more detailed description can be found in the cited references.

The EOS of the van der Waals gas is

$$P(\rho, \epsilon) = (\gamma - 1) \frac{\rho \epsilon + a \rho^2}{1 - b \rho} - a \rho^2, \tag{4.1}$$

where γ , a and b are constant. We decompose the EOS of the van der Waals gas as

$$P_1(\rho, \epsilon) = (\gamma - 1) \frac{\rho \epsilon + a \rho^2}{1 - b \rho} - a \rho^2, \quad P_2(\rho, \epsilon) = 0. \tag{4.2}$$

Therefore, with the phase evolving variables chosen as in the end of Section 2, the partial pressure of the k th fluid in the i th cell is computed by

$$p_{k,i} = (\gamma_{k,i} - 1) \frac{\rho_{k,i} \epsilon_{k,i} + a_k \rho_{k,i}^2}{1 - b_k \rho_i} - a_k \rho_{k,i}^2, \tag{4.3}$$

if the fluid is van der Waals.

The CFL number is always set as 0.5. For each example we present the numerical results of the mixture density, velocity, mixture pressure and total energy. In all the following figures we use solid lines to represent the exact solutions and use dots for the numerical solutions. Because of the heavy dissipation of the LxF scheme, very fine grids are used in all the tests. In the end of this section, we present a numerical solution computed with the second-order extension of the LxF scheme to show the improvement.

4.1 Numerical tests

Test 4.1. The initial value is

$$\begin{cases} 0 < x < 0.5, & 0.5 < x < 1.0, \\ \rho_l = 1.0, & \rho_r = 0.125, \\ u_l = 0.0, & u_r = 0.0, \\ p_l = 1.0, & p_r = 0.1, \\ \gamma_l = 1.6, & \gamma_r = 1.2. \end{cases} \quad (4.4)$$

The problem is chosen from [1]. The numerical solution on a grid of 1,000 cells at $t = 0.25$ is presented in Fig. 1.

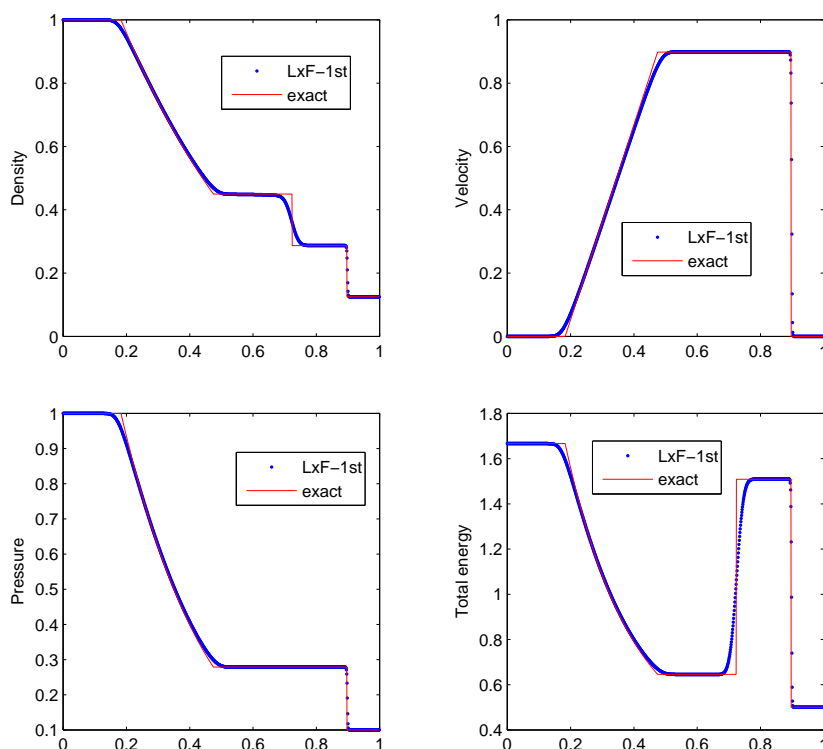


Figure 1: Numerical solution of Test 4.1 at $t = 0.25$, 1,000 grid cells.

Test 4.2. The initial value is

$$\begin{cases} 0 < x < 2.0, & 2.0 < x < 4.0, & \rho_l = 10^{-\frac{6.0}{7.0}}, & \rho_r = 1.0, \\ u_l = 0.0, & u_r = 0.0, & p_l = 10^3, & p_r = 1.0, \\ \gamma_l = 1.4, & \gamma_r = 7.0, & \mathcal{B}_r = 3000, & \rho_0 = 1.0. \end{cases} \quad (4.5)$$

The problem is chosen from [11]. The left gas is polytropic and the right gas is barotropic. The numerical solution on a grid of 1,000 cells at $t = 0.01$ is presented in Fig. 2.

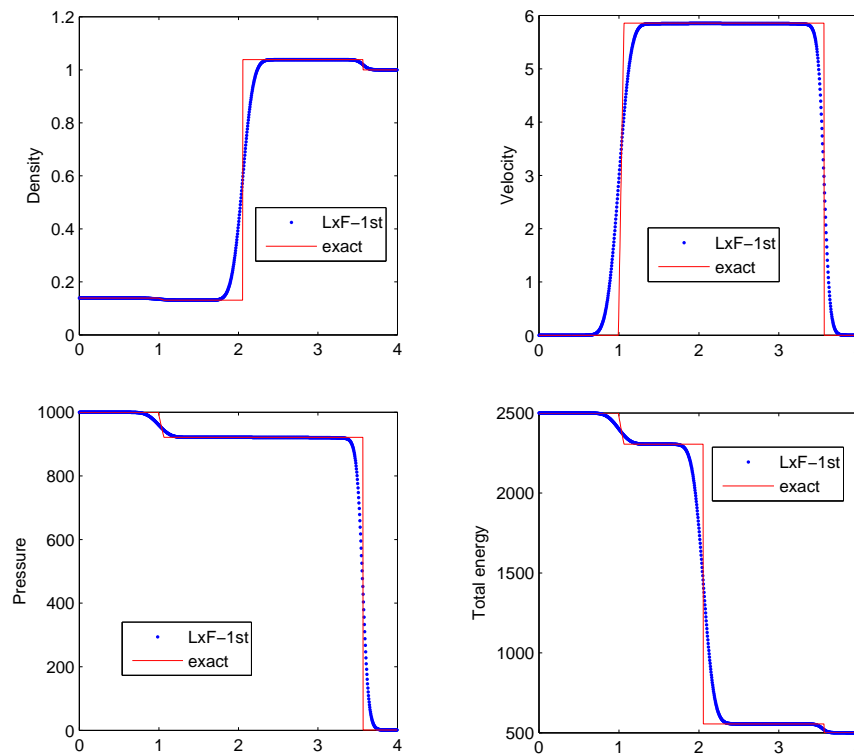


Figure 2: Numerical solution of Test 4.2 at $t = 0.01$, 1,000 grid cells.

Test 4.3. The initial value is

$$\begin{cases} 0 < x < 0.5, & 0.5 < x < 1.0, & \rho_l = 10^3, & \rho_r = 50, \\ u_l = 0.0, & u_r = 0.0, & p_l = 10^9, & p_r = 10^5, \\ \gamma_l = 4.4, & B_l = 600,000,000, & \gamma_r = 1.4. \end{cases} \quad (4.6)$$

The problem is chosen from [1]. The left gas is stiffened and the right gas is polytropic. Numerical solution on a grid of 10,000 cells at $t = 0.0001$ is presented in Fig. 3.

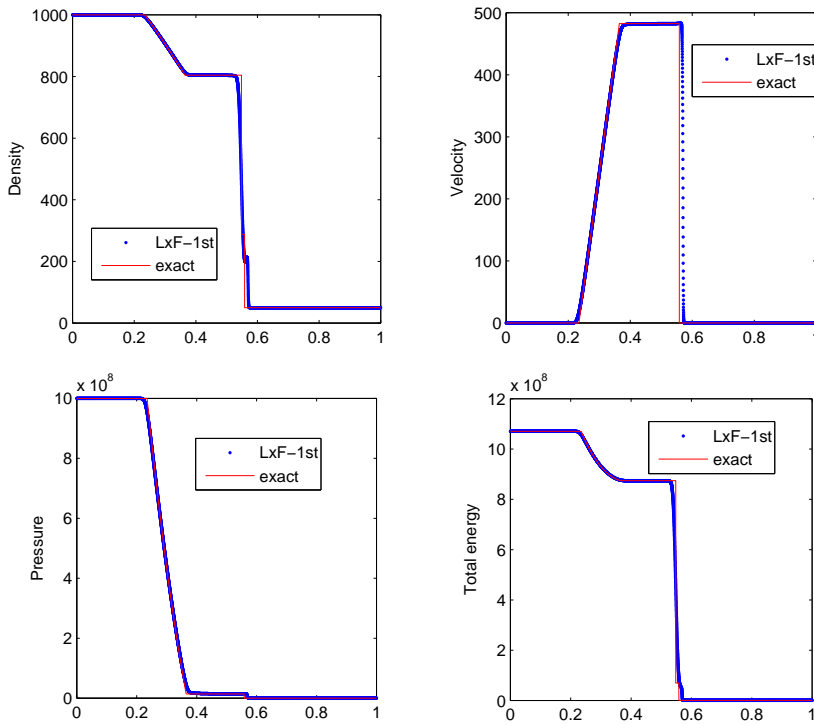


Figure 3: Numerical solution of Test 4.3 at $t=0.0001$, 10,000 grid cells.

Test 4.4. The initial value is

$$\begin{cases} 0 < x < 1.0, & 1.0 < x < 2.0, & \rho_l = 10^3, & \rho_r = 50.0, \\ u_l = 0.0, & u_r = 0.0, & p_l = 10^9, & p_r = 10^5, \\ \gamma_l = 4.4, & \mathcal{B}_l = 600,000,000, & \gamma_r = 1.4, & a_r = 5.0, & b_r = 1.0^{-3}. \end{cases} \quad (4.7)$$

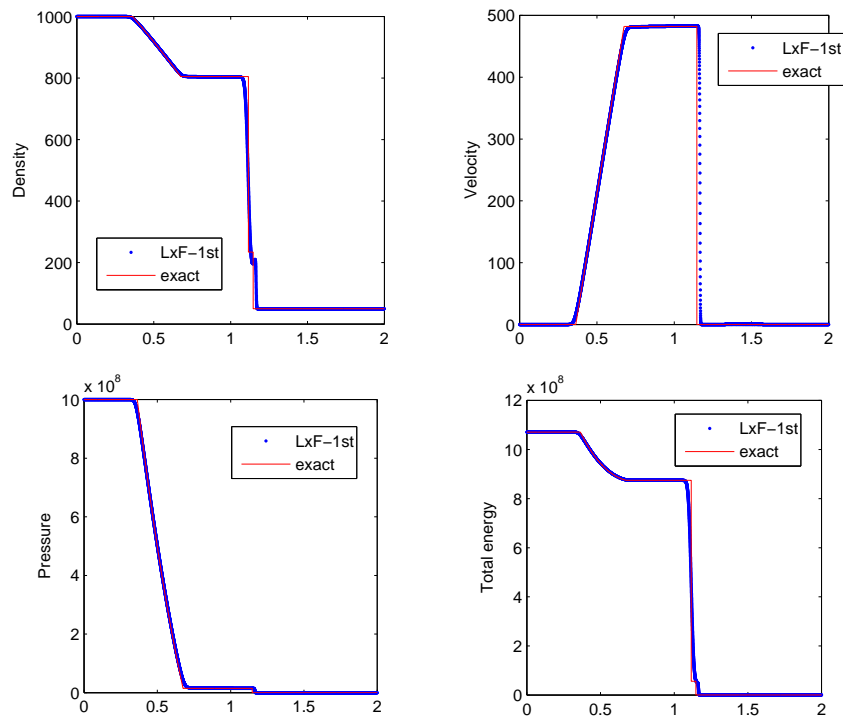
The problem is chosen from [10]. the left gas is stiffened and the right gas is van der Waals. Numerical solution at $t=0.00024$ on a grid of 10,000 cells is presented in Fig. 4.

As is described in the beginning of this section, the partial pressure of the van der Waals gas is computed as in (4.3). However, in this test the mixture density will reach 1,000 in cells on the left of the interface where the stiffened gas is dominated, which will cause the denominator $1 - b_r \rho_i$ in (4.3) to approach zero. To fix the problem, we set

$$\bar{\rho}_i = \min \left\{ \rho_i, \frac{0.8}{b_r} \right\}, \quad (4.8)$$

and then compute the partial pressure contributed by the van der Waals fluid, $p_{W,i}$, as

$$p_{W,i} := \frac{(\gamma_r - 1)(\epsilon_{2,i} \rho_{2,i} + a_r \rho_i \bar{\rho}_{2,i})}{1 - b_r \bar{\rho}_i} - a_r \bar{\rho}_i \rho_{2,i}, \quad (4.9)$$

Figure 4: Numerical solution of Test 4.4 at $t=0.00024$, 10,000 grid cells.

with ρ_i replaced by $\bar{\rho}_i$. Note, this fix does not affect the conservation of the individual masses, mixture momentum and mixture energy; it only alters a bit the computation of the two partial energies near the interface. The fix corresponds to introduce some numerical energy exchange between the two fluids.

4.2 Observations and comments

Generally speaking, all the numerical solutions are in good agreement with the exact solutions, and as expected, the velocities and pressures of the fluid mixture experience little fluctuations across the interfaces, even for the van der Waals gas in Test 4.4, which does not have the UPV property guaranteed by Theorem 3.2. This indicates that the proposed model and its LxF scheme are efficient and able to treat fluids characterized with a wide range of different thermodynamics.

It is obvious that all the numerical solutions suffer from the heavy numerical dissipation of the LxF scheme. A second-order extension of the scheme in the ways of [7] has been built and a separate paper will be devoted to that issue. Nevertheless, we would like to present in Fig. 5 the numerical solution computed by the second-order scheme on a grid of 100 cells for Test 4.1 and compare it with the numerical solution computed by the first-order scheme on the same grid. The improvement of the second-order scheme over the first-order one is clearly seen in the figure.

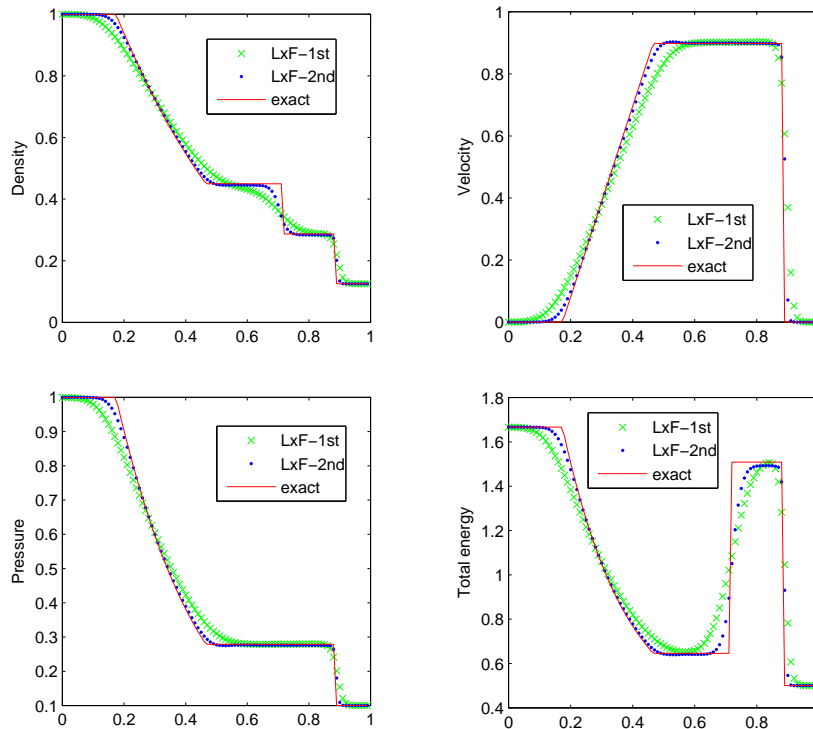


Figure 5: Numerical solutions of Test 4.1 computed by the first- and second-order LxF schemes at $t=0.25$, 100 grid cells.

We note that the numerical solutions in Tests 4.3 and 4.4 do not quite converge to the exact solutions; the right shocks do not travel at correct speeds and the densities have undershoots behind the interfaces. We guess the problem is caused by that all the tests involve a very stiffened gas ($\mathcal{B}_l = 600,000,000$) and have great jumps in both density and pressure; therefore, the problems similar to that reported in [13] for single fluids take place in these tests, and this kind of problems may be severed in simulations of two-fluid flows.

5 Conclusions

We have presented a modified BN model and a corresponding LxF scheme for a particular case of the model. The modification is mainly on the energy exchange in the work done by the pressure. Also the mixture pressures is computed in a generalized way in which four sets of phase evolving variables are used to describe the thermodynamics of the fluid mixture. The model consists of eleven equations; however, particular choices of the phase evolving variables reduce the model to have only six equations. The model and the LxF scheme are hyperbolic and maintain the conservation of individual masses, momentum and total energy. Also the model and the LxF scheme meet the UPV criterion

for linear Mie-Gruneisen fluids. Numerical experiments show that the model and the LxF scheme are efficient and able to handle fluids characterized with different thermodynamics.

Acknowledgments

The authors would like to thank the referee for his valuable comments and suggestions, which lead to several revisions and modifications of the original manuscript of the paper. The research is supported by China National Science Foundation Grant No. 10971132, Leading Academic Discipline Project of Shanghai Municipal Education Commission No. J50101 and Shanghai Pu Jiang program [2006] 118.

References

- [1] R. Abgrall and S. Karni, Computations of compressible multifluids, *J. Comput. Phys.*, 169 (2001), 594–623.
- [2] M. R. Baer and J. W. Nunziato, A two-phase mixture theory for the deflagration-to-detonation transition (DDT) in reactive granular materials, *Int. J. Multiphase. Flow.*, 12 (1986), 861–889.
- [3] J. B. Bdzil, R. Menikoff, S. F. Son, A. K. Kapila and D. S. Stewart, Two-phase modeling of deflagration-to-detonation transition in granular materials: a critical examination of modeling issues, *Phys. Fluids.*, 11 (1999), 378–402.
- [4] J. B. Bdzil, R. Menikoff, S. F. Son, A. K. Kapila and D. S. Stewart, Two-phase modeling of deflagration-to-detonation transition in granular materials: reduced equations, *Phys. Fluids.*, 13 (2001), 3002–3024.
- [5] D. Drew, Mathematical modeling of two-phase flow, *Ann. Rev. Fluid. Mech.*, 15 (1983), 261–291.
- [6] A. Muronne and H. Guillard, A five equation reduced model for compressible two phase flow problem, *J. Comput. Phys.*, 202 (2005), 664–698.
- [7] H. Nessyahu and E. Tadmor, Non-oscillatory central-differencing for hyperbolic conservation laws, *J. Comput. Phys.*, 87 (1990), 408–463.
- [8] P. Saurel and R. Abgrall, A multiphase Godunov method for compressible multifluid and multiphase flows, *J. Comput. Phys.*, 150 (1999), 425–467.
- [9] P. Saurel and R. Abgrall, A simple method for compressible multifluid flows, *SIAM J. Sci. Comput.*, 21 (1999), 1115–1145.
- [10] Keh-Ming Shyue, A fluid-mixture type algorithm for compressible multicomponent flow with Van der Waals equation of state, *J. Comput. Phys.*, 156 (1999), 43–88.
- [11] Keh-Ming Shyue, A fluid-mixture type algorithm for barotropic two-fluid flow problems, *J. Comput. Phys.*, 200 (2004), 718–748.
- [12] Keh-Ming Shyue, A fluid-mixture type algorithm for compressible multicomponent flow with Mie-Gruneisen equation of state, *J. Comput. Phys.*, 171 (2001), 678–707.
- [13] H. Tang and T. Liu, A note on the conservative schemes for the Euler equations, *J. Comput. Phys.*, 218 (2006), 451–459.
- [14] C. Wang, The Lax-Friedrichs Scheme for Multifluid Flows, MSc. Thesis (in Chinese), Shanghai University, No. 23140103720678.