# Study on New Methods for Accurate Modeling of Energy Equation with Multi Species

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**Abstract:** In this work, we developed a finite volume method code to handle the flow field problem of the one-dimensional unsteady Euler equations caused by the moving contact discontinuity interface between two different species on both sides of the shock tube. The derived additional energy conservation equation introduces a non-conservative term. It is crucial to reduce non-physical numerical oscillations and enhance shock-capturing capability and computational accuracy, especially for high-resolution problems. In this study, firstly, we extended the energy equation of the unsteady Euler equations to accommodate *i* species and considered different state equations. Based on the test results, it was found that the considered state equations did not improve the above issues. Furthermore, we attempted to extend the first-order flux limiter to second order and tested its effectiveness. The results showed that the quadratic term had minimal impact on the entire computation process in gradient calculations. Hence, attempting to improve the flux limiter through this approach was deemed inappropriate.

**Keywords:** Euler equations, numerical oscillation, contact discontinuity, shock capturing, Runge-Kutta method, gradient method, flux limiter

## 1. Introduction

In 1984, the flux vector questions of Euler equations for compressible flow with consideration of the simplest and ideal gas laws, Leer [1] discussed the type of shock wave under the steady state between two regions based on first order upwind scheme. In addition, the problems of supersonic un-differential point and stagnation point, we treated this kind question with the type of split fluxes has the equivalent advantage according to the form developed by Steger and Warming [2].

Dealing with the Riemann problem of unsteady hypersonic flow, directly solving the conservation equations numerically poses difficulties due to non-linear phenomena. In the 1950s, Godunov [3] suggested using previous time point information for accurately solving discretized conservation equations of a single ideal gas. In 1979, Leer developed the second-order extenmon of Godunov's method for hyperbohc conservatton laws, known as MUSCL method and the Total Variation Diminishing (TVD) scheme for high-order accuracy in numerical computing. Detailed wave system approximations are found in Roe [4] and Osher [5] solvers; Roe's solver uses local linearization [6], while Osher's replaces shock waves with simple compression waves, known as "flux-difference splitting". In 1994, Wada and Liou [7] proposed the A Flux Splitting Scheme (AUSMDV) method, improving upwind split schemes based on the Advection Upstream Splitting Method (AUSM) principle. Combining numerical flux with flux limiters improves computation accuracy and prevents violent oscillations, especially at shock waves and contact discontinuities.

## 2. Modelling

In this study, we consider 1D-Euler equations with gas mixture model in general form,

$$\frac{\partial}{\partial t}\int_V Udx + \int_{\partial V} FdA = \int_V Qdx, \tag{1}$$

where $V$ stands for volume, $U$ is the vector relation of conservation variables, $\partial V$ represents surface, $F$ is frictionless flux vector and $Q$ depicts the vector parameter of source terms, see Shieh and Li [8] as well as Shieh *et al.* [9]. Those vector parameters could be defined as

$$U = [\rho_i, \rho u, \rho_i E_i, \rho E], F = [\rho_i u, \rho u^2 + P, \rho_i E_i u, \rho E u + Pu], Q = [0, 0, -(u_i P_i)_x + [\rho_i E_i (u - u_i)]_x, 0]. \tag{2}$$

We let "Model $B_1$" be the expression form Eq. (2) and "Model $B_2$" be the form as

$$Q = [0, 0, -(u_i P_i)_x + \rho_i E_i (u - u_i)_x, 0]. \tag{3}$$

In addition, "Model $B_3$" is displayed by

$$Q = [0, 0, -(u_i P_i)_x, 0]. \tag{4}$$

Based on gas mixture, the third vector describes the additional energy source term which Ton [10] expand it. Therefore, the different two densities $\rho_1$ and $\rho_2$ just get the energy of other species from the total energy and produce an extra individual energy $\rho_1 E_1$. In the above vector matrices, mixing specific heat ratio $\gamma$ is simplified as

$$\gamma = 1 + \left[\sum_{i=1}^{ns}(Y_i/W_i) \Big/ \sum_{i=1}^{ns}\big(Y_i/W_i\,(\gamma_i - 1)\big)\right].$$

Moreover, the thermodynamic function among the individual pressure $P_i$ , energy $E_i$ and specific heat ratio $\gamma_i$ is shown as $P_i = (\gamma_i - 1)\left(\rho_i E_i - \frac{1}{2}\rho_i u^2\right)$.

## 3. Numerical Method

### 3.1. Finite Volume Method

By the discretization of Eq. (1), we classify the computational domain to the distinct control volume $K$, where the boundary of individual computing cells could be defined by mesh border. We transform the difference equation into an algebraic equation by integrating along the computing cells. Eq. (1) using closed volume between $\Delta t$ and $\Delta x$. Now, for the computing cell boundary, we again consider the form of conservation equations as

$$\frac{\partial}{\partial t}\int_K U(x,t)dx + \oint_{\partial K} F(x,t)dA = \int_K Q(x,t)dx.$$

The variable $\phi_K$ is defined by $\phi_K(t) := \int_K Q(x,t)dx - \oint_{\partial K} F(x,t)dA$.

Through the flux calculation in AUSMDV Riemann solver and the discretization of source term $Q(x,t)$ , the individual control volume $K$ is defined by the mean value $U$ of every grid. For 1D space discretization, we can get a discretized form of first order time stepping by

$$\Delta\overline{U_K} = \overline{U_K}(t_2) - \overline{U_K}(t_1), \Delta\overline{U_K}(x,t_2) = \overline{U_K}(x,t_1) + \frac{\Delta t}{\Delta x}\phi_K(x,t_s). \tag{5}$$

Through the process of temporal iterations, we solve the variables of temporal discretization in every volume mesh after the previous temporal and space discretization.

### 3.2. Time Stepping Procedure

In the presenting study, the explicit method is applied to deal with the time discretization of Eq. (1). For the time stepping procedure, we recall the Eq. (5) to obtain the following explicit two-steps second-order Runge-Kutta method with

$$U_K(x,t_2) \approx U_K(x,t_1) + \frac{\Delta t}{2\cdot\Delta x}\phi\big(U_K(x,t_1)\big)$$
$$+\frac{\Delta t}{2\cdot\Delta x}\phi\left[U_K(x,t_1) + \frac{\Delta t}{\Delta x}\phi\big(U_K(x,t_1)\big) + \frac{\Delta t^2}{2!\cdot\Delta x}\phi^2\big(U_K(x,t_1)\big)\right].$$

## 4. Results

In this study, we mainly carried out a series of tests for the new additional energy term in the condition of dual gas. Then we considered the simplest two gases to carry out tests. The classification of our study is expressed as Table 1.

Table 1. The Initial Condition of the Reference Solution

| | $\Delta x$ | $C_{CFL}$ | Limiter | Integration |
|---|---|---|---|---|
| Reference solution | 0.0001 | 0.9 | van Leer | Second-order Runge-Kutta method |

Additionally, we applied two species which are air and helium (He) separately, and the foundational parameters of the species are given in Table 2. On the other hand, the boundary conditions are set as: (i) the stepping size of the space discretization $\Delta x = 0.01$, (ii) the stability factor $C_{CFL} = 0.9$ and (iii) the maximal timesteps equal to 20,000. Here, we adopt the first-order backward ($B^1$) difference method. Taking the initial conditions in Table 3, we verified the ability of through the test condition of dual species. In this case, we tested the influence of the varied forms of EOS for the additional energy term.

Table 2. The Thermodynamic Parameters of Test Species

| | $W$ | $R$ | $\gamma$ |
|---|---|---|---|
| Air | 28.97 | 0.287 | 1.4 |
| He | 4.003 | 2.0769 | 1.667 |

Table 3. The Dual Species Initial Condition of the Shock Tube Problem

| Air | $\rho_1$ | $\rho_2$ | $u$ | $P$ | $Y_1$ | $Y_2$ | $x$ |
|---|---|---|---|---|---|---|---|
| Species condition of left-hand side (L) | 1 | 0 | 0 | 1 | 1 | 0 | $x < 0.5$ |
| Species condition of right-hand side (R) | 0 | 0.8 | 0 | 0.2 | 0 | 1 | $x \geq 0.5$ |

- $P_{normal}$: We computed the additional source term $Q$ by the relation form of pressure $P$, $P_i = (\gamma_i - 1)\left(\rho_i E_i - \frac{1}{2}\rho_i u^2\right)$.
- $P_{M.E}$: We considered the velocity of individual species and try to substitute for the velocity $u$ by the specific velocity $u_i$. Then the relation form of pressure is expressed as $P_i = (\gamma_i - 1)\left(\rho_i E_i - \frac{1}{2}\rho_i u_i^2\right)$.

After that, we carried out the simulation through the dual-gas initial condition of shock wave and adopting the first order difference method and Superbee limiter to discuss whether the estimation ability can be improved by this way.

By Fig. 1, the numerical oscillations are somehow improved for Model $B_1$ and $B_2$, and the perpendicularity of Model $B_3$ seems to become better. Further, we observed the others related diagrams, Figs. 2–4, the non-physical oscillations of Model B1 becomes little better but its catching capability gets worse more. However, for Model $B_2$ and $B_3$, not only the oscillations get grievous but their capturing-shock abilities are more and worse. For example, in Fig. 2, the numerical oscillations of $B_2$ and $B_3$ occur when the velocity changes around $x = 0.65$ and the numerical results depart from shock wave. For Fig. 4, the variation inclinations are similarly to $P$-related figure. Hence, we knew there are no benefits for considering $P_i$ for $P_{M.E}$. Maybe we could try other forms of equation of state.

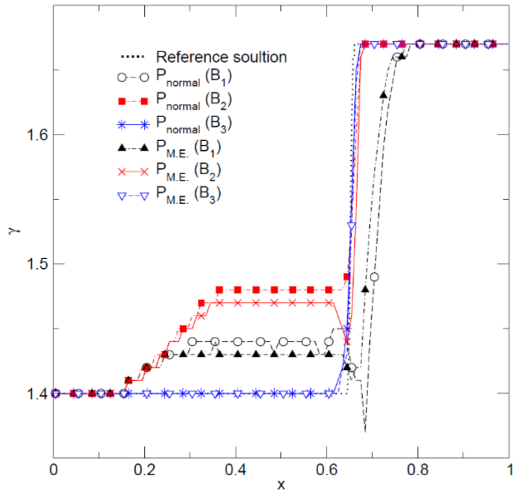


Fig. 1. $\gamma$-related figure of the different EOS for new models.

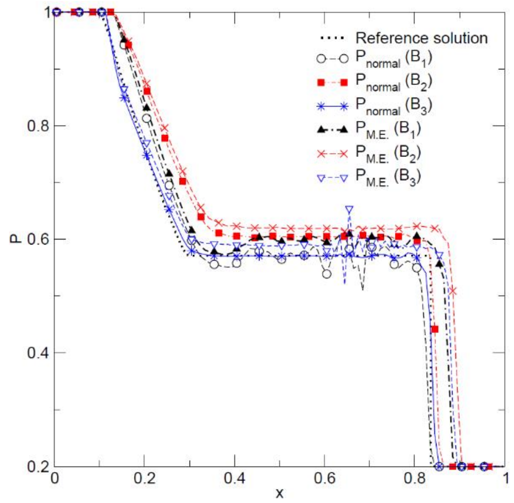


Fig. 2. $P$-related figure of the different EOS for new models.

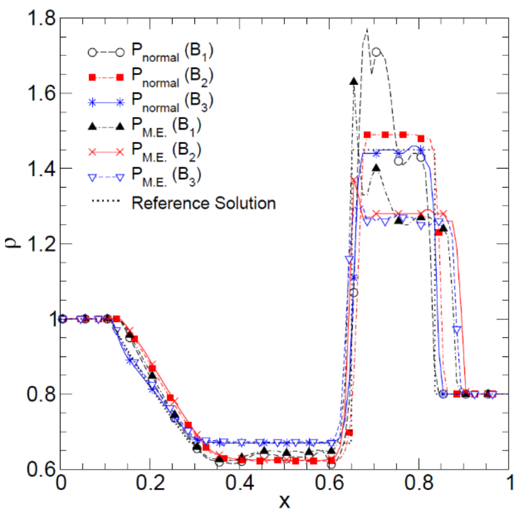


Fig. 3. $\rho$-related figure of the different EOS for new models.

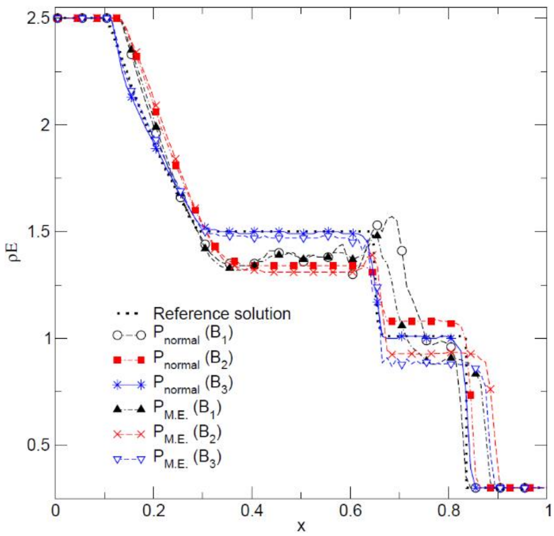


Fig. 4. $\rho E$-related figure of the different EOS for new models.

In the time stepping dissemination of one-dimensional system follows the principle of Riemann average variable. The restriction function is inferred from the restriction factor $\varphi$ based on the one-side gradient of neighbor grid, and the gradient must be increase with the step of numerical reconstruction. In general, the judgement in both sides of grid adds the restriction function by using approximate piecewise linear method for the TVD scheme. However, we expanded the first-order restriction expression to the second-order relation form. And then, we used the initial condition of dual mix gas for the new derived energy Model $B_3$ joining the $B^1$ difference method and $\mathrm{RK}_2$ scheme to examine the effect that the limit function adds the quadratic term.

According to the related diagrams of $\rho$ and $u$, Figs. 5–8, the numerical consequences which have the square term in limit expression have not evident diversity; further, they are almost identical compared with that without the square expression. Originally, we expected that the perpendicularity on the region of high gradient is improved through the quadratic to adjust its computing ability. However, apparently, the outcomes show that the value of quadratic term is quite slight such that it is no use for the entire process of simulation.

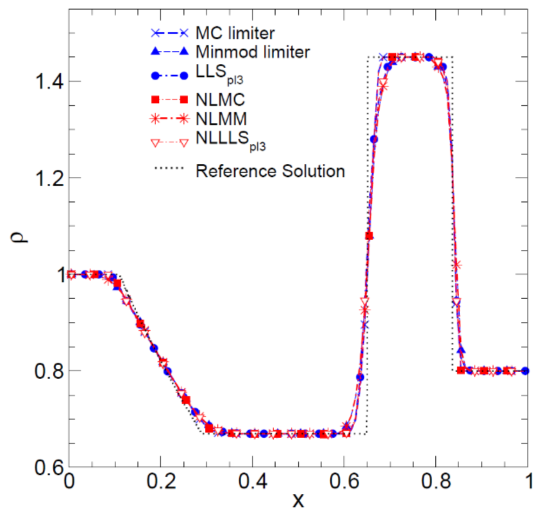


Fig. 5. $\rho$-related figure of the comparison for second-order estimation of gradient in flux limiter.

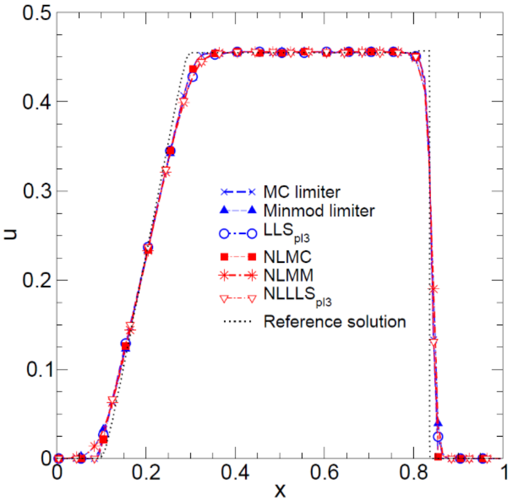


Fig. 6. $u$-related figure of the comparison for second-order estimation of gradient in flux limiter.

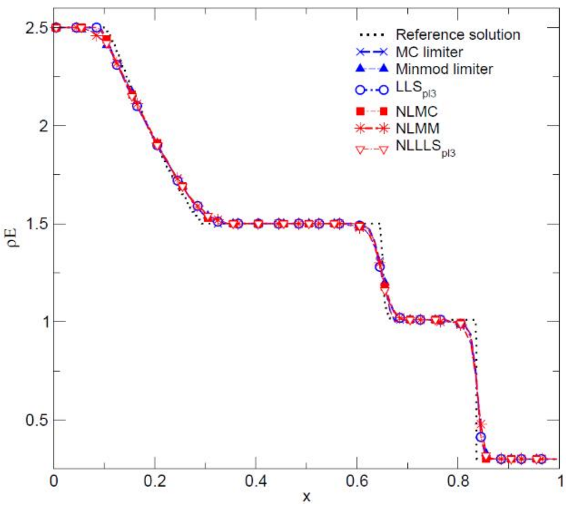


Fig. 7. $\rho E$-related figure of the comparison for second-order estimation of gradient in flux limiter.

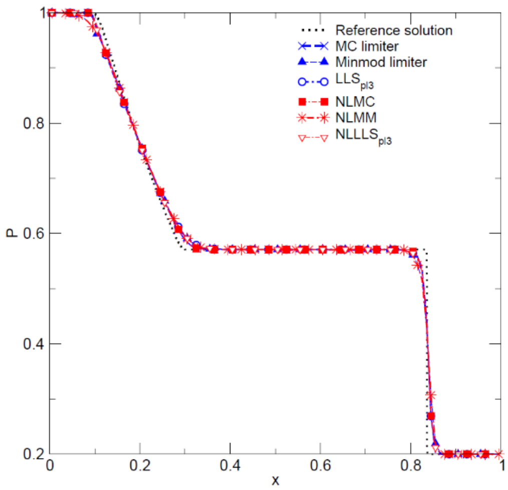


Fig. 8. $P$-related figure of the comparison for second-order estimation of gradient in flux limiter.

## 5. Conclusion

We wanted to know the influence of the varied forms of EOS for the additional energy term, so we considered the specific velocity $u_i$ into the Equation of State (EOS) to test its computing precision. Then we did simulation through the dual-gas condition of shock wave and using the $B^1$ difference method and Superbee limiter to discuss whether the estimation ability can be improved by this manner. As the testing results, not only the oscillations of Model $B_3$ get grievous but its capturing-shock abilities are more and more unhealthy. Hence, we knew that it is no uses through considering the case of $P_{M.E}$, or maybe we should say that the considered EOS is inappropriate for our test case. As the second test results, we got that the influence of the quadratic term of gradient estimation is insignificant, even almost no, for the whole computing procedure. Hence, that we wanted to improve the flux limiters through this way is unsuitable.

## Conflict of Interest

The authors declare no conflict of interest.

## Author Contributions

The first author's contributions to this work include methodology, validation, formal analysis, and writing. The corresponding author provided review and supervision. All authors have approved the final version.

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