Detonation Simulations with a Fifth-Order TENO Scheme

Haibo Dong¹, Lin Fu², Fan Zhang³,* , Yu Liu⁴ and Jun Liu¹

¹ State Key Laboratory of Structural Analysis for Industrial Equipment, Dalian University of Technology, Dalian 116024, China.
² Center for Turbulence Research, Stanford University, Stanford, CA 94305, USA.
³ School of Aeronautics and Astronautics, Sun Yat-sen University, Guangzhou 510006, China.
⁴ Department of Aerospace Science and Technology, Space Engineering University, Beijing 101416, China.

Received 10 January 2018; Accepted (in revised version) 27 June 2018

Abstract. In [Fu et al., JCP 305(2016): 333-359], a family of high-order targeted ENO (TENO) schemes is proposed. The weighting strategy of TENO either applies a candidate stencil with its optimal weight, or removes its contribution completely when it is crossed by discontinuities. This ENO-like stencil selection procedure significantly diminishes the numerical dissipation induced by the nonlinear adaptations of classical WENO schemes. In this paper, the fifth-order TENO scheme is extended to simulate reactive flows in combination with an uncoupled method [1, 2], which splits the reaction source term of detailed chemistry from the flow equations. A set of benchmark cases including the two-dimensional self-sustained detonation is simulated to validate and compare the performance of the fifth-order WENO and TENO schemes. Numerical experiments demonstrate that TENO scheme is robust for simulating chemical reacting flows with using the uncoupled method. In particular, TENO scheme shows better performance in capturing both the shockwaves and the small-scale flow structures, e.g. shear layers and vortices.

AMS subject classifications: 35L65, 65M06, 76J20, 76V05
Key words: WENO, TENO, chemical reacting flow, uncoupled method, shockwave; detonation.

1 Introduction

Detonations are supersonic combustion, where the combustion fronts interact with strong leading shockwaves. During a detonation, the combustible or reactive material, e.g. gas

*Corresponding author. Email addresses: donghaibo@mail.dlut.edu.cn (H. B. Dong), linfu@stanford.edu (L. Fu), zhangfan3@mail.sysu.edu.cn, a04051127@mail.dlut.edu.cn (F. Zhang), liuyu@nudt.edu.cn (Y. Liu), liujun65@dlut.edu.cn (J. Liu)
fuel, is ignited by the high temperature and pressure. Moreover, the exothermic process of the chemical reactions releases massive energy which further increases the post-shock temperature and pressure, and eventually drives the shockwaves moving to unreacted regions. While the complicated mechanism of self-sustained detonation is interesting with regard to the point of view of fluid dynamics, detonation is extensively investigated for improving the performance of air-breathing combustion engine [3]. Consequently, the development of numerical methods for detonation simulations is an attractive topic in the past decades.

For multi-dimensional detonations, it is proved that numerical simulations play a significant role to elucidate the flow instabilities and the complex flow structures [4, 5]. The solution qualities may be affected by several important numerical issues, e.g. the chemical reaction model [6], the temporal/spatial discretization [7, 8] and the solution of chemical source term [9, 10]. Moreover, several strategies [11, 12] have been proposed to solve the coupling systems of reactive flow equations. An uncoupled method [1, 2] following the idea of Strang splitting [13] can be applied to split the solution of detailed chemistry from the solution of the spatial terms of flow governing equations, and more improvements and/or applications of this method were introduced in several articles [8, 14–16]. In this way, the spatial discretization methods and the chemical reaction solvers can be investigated and developed separately.

Nevertheless, for detonation simulations, developing a high-resolution method to solve the governing equations accurately is still a challenge. The popular second-order finite-volume (FV) method with multi-resolution meshes [17, 18] has shown great potentials. However, since the flow structures in detonations are rather complicated, high-order (third-order or higher) schemes can be useful for resolving delicate flow structures. For example, sufficient resolution is necessary to capture detonation structures [5], e.g. triple point(s), and hydrodynamic instabilities [19–21] may play important roles during the onset and evolution of detonations [22–24] or combustion [25, 26], leading to high demand for numerical accuracy [27]. A more specific situation is that in the simulation of high activation energy gas, high resolution is required to correctly resolve the mixing rate in the flow field, which affects the strength of detonation wave or combustion [28].

Weighted essentially non-oscillatory (WENO) schemes [29], the weights of which are designed to recover the ENO property [30] for capturing discontinuities and to restore the background linear schemes in smooth regions, is extended to solve reactive flows because of its high-resolution property.

The fifth-order WENO-JS scheme [31] has been employed to study the cellular detonation in a straight tube [32], and the self-sustained cellular detonation is well captured. However, the classical WENO-JS scheme fails to recover the formal fifth-order accuracy near critical points, where low-order derivatives vanish. Henrick et al. [33] proposed the WENO-M scheme which maps the WENO-JS weights such that the sufficient criteria for restoring the fifth-order accuracy is suggested to be satisfied. The WENO-M scheme has been applied to simulate detonation phenomena in combination with the uncoupled method [2] within the finite-difference (FD) framework [34]. Borges et al. [35]
found that the improvement of WENO-M scheme for shock-capturing is mainly due to
the larger weights assigned to the nonsmooth stencils, and WENO-Z scheme is proposed
and shows high-order accuracy even at critical points. Later, WENO-Z scheme and its im-
provement have been well studied in two- and three- dimensional detonations [36,37].
Hybrid central-WENO schemes [24,38,39] have also been developed to capture the multi-
scale flow structures of detonations and combustion.

Despite the celebrating success of WENO schemes in simulating detonations and
other reactive flow problems, there are several typical drawbacks. For instance, clas-
sical WENO schemes are unnecessarily dissipative for resolving small-scale structures.
Various improved versions [33,35] of WENO schemes are proposed to fix these issues.
Moreover, there are several researches [40,41] that design new discontinuity detectors to
exploit the low dissipation property of the linear scheme and to capture shockwaves by
using WENO scheme. Recently, a new family of ENO type scheme, i.e. TENO scheme,
is proposed by Fu et al. [42] and shows outstanding performance in resolving interme-
diate and high-wavenumber physical fluctuations. The TENO scheme maintains the op-
timal weights to recover the background linear upwind scheme in smooth regions and
removes the oscillating reconstruction by completely excluding those stencils crossing
discontinuities, instead of changing the corresponding nonlinear weights. Moreover, the
incremental candidate stencils of TENO scheme improve its capability in handling mul-
tiple discontinuities close to each other. In [43], a new sixth-order TENO8-opt scheme is
constructed by employing the background linear scheme which has optimized dispersion
and minimum dissipation that satisfy an approximate dispersion relation. Benchmarks
with broadband fluctuations are computed to demonstrate the high-resolution properties
of the TENO8-opt scheme. Since the great potential of TENO family schemes in better
resolving the multi-scale flow structures is shown, it is expected that TENO schemes can
perform better than classical WENO schemes in simulating chemical reacting flows.

In this paper, a chemical reaction solver with using TENO scheme [42] for spatial re-
construction and the uncoupled method [1, 2] for splitting the source terms of detailed
chemistry is developed. The remainder of this paper is organized as follows. In Section
2, a brief review of WENO and TENO schemes for the one-dimensional scalar hyper-
bolic conservation law is given. In Section 3, the governing equations and the formula of
splitting method are outlined in detail. Numerical experiments of thermally perfect gas
and gaseous mixture denotation are presented in Section 4 to assess the performance of
TENO scheme. Conclusions and remarks will be given in the last section.

2 Hyperbolic conservation law and TENO scheme

The chemical reaction problem is governed by a hyperbolic system with a stiff source
term. Therefore, without loss of generality, WENO schemes and TENO scheme are intro-
duced based on the one-dimensional scalar hyperbolic conservation law, and the schemes
can be extended to hyperbolic system equations straightforwardly. In this paper, only
typical five-point stencil schemes are discussed and applied.
2.1 Fundamental of WENO schemes

The one-dimensional hyperbolic conservation law that describes the essential property of hyperbolic system such as the governing equations of compressible aerodynamics, is written as

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \quad (2.1)$$

in which the characteristic velocity is $\frac{\partial f(u)}{\partial u}$ and can be assumed to be positive, without loss of generality. For simplicity, the spatial discretization of Eq. (2.1) is given on an uniform one-dimensional mesh, leading to an ODE (ordinary differential equation) system, i.e.

$$du_i dt = -\frac{\partial f}{\partial x} |_{x=x_i}, \quad i = 1, \ldots, n. \quad (2.2)$$

The partial derivatives in $x$-direction are approximated by using the finite difference formula as

$$du_i dt = -\frac{1}{\Delta x}(h_{i+1/2} - h_{i-1/2}). \quad (2.3)$$

The flux function $h_{i\pm1/2}$ at half points can be implicitly defined by

$$f(x) = \frac{1}{\Delta x} \int_{x-\Delta x/2}^{x+\Delta x/2} h(\xi) d\xi, \quad (2.4)$$

and the semi-discretized form can be further written as

$$du_i dt \approx -\frac{1}{\Delta x}(\hat{f}_{i+1/2} - \hat{f}_{i-1/2}), \quad (2.5)$$

where the numerical flux functions $\hat{f}_{i\pm1/2}$ are calculated from the convex combination of $r$ candidate-stencil fluxes

$$\hat{f}_{i\pm1/2} = \sum_{k=0}^{r-1} \omega_k \hat{f}_{k,i\pm1/2}. \quad (2.6)$$

In order to obtain a $(2r-1)$-order approximation for flux functions $\hat{f}_{i\pm1/2}$, a $(r-1)$-order interpolation on each candidate stencil is given as

$$h(x) \approx \hat{f}_k(x) = \sum_{l=0}^{r-1} a_{l,k} x^l, \quad (2.7)$$

where the coefficients $a_{l,k}$ can be calculated by substituting Eq. (2.7) into Eq. (2.4) and solving the resulting linear algebraic system. However, the solution or design of the weight, $\omega_k$, is the challenging part in the research of WENO schemes, and will be introduced in the following sections.

Eventually, based on the spatial approximation of the flux function, the temporal differential term in the ODE system Eq. (2.2) can be solved by using the third-order TVD Runge-Kutta method [44].
2.2 WENO-JS scheme

For the classical fifth-order WENO-JS scheme [31], of which \( r = 3 \), two-degree polynomial approximation of the numerical flux function can be given as

\[
\hat{f}_k(x) = a_{0,k} + a_{1,k}x + a_{2,k}x^2,
\]

which is capable to give third-order accuracy approximation. Specifically, the numerical flux functions of the candidate stencils for the approximation at grid half point \( i + \frac{1}{2} \) are

\[
\begin{align*}
\hat{f}_{0,i+1/2} &= \frac{1}{6}(2f_{i-2} - 7f_{i-1} + 11f_i), \\
\hat{f}_{1,i+1/2} &= \frac{1}{6}(-f_{i-1} + 5f_i + 2f_{i+1}), \\
\hat{f}_{2,i+1/2} &= \frac{1}{6}(2f_i + 5f_{i+1} - f_{i+2}).
\end{align*}
\]

The error of the approximation in Eq. (2.9) can be obtained by Taylor expansion analysis, i.e.

\[
\hat{f}_{k,i+1/2} = h_{k,i+1/2} + C_k\Delta x^3 + O(\Delta x^4), \quad k = 0, 1, 2.
\]

Thereinto, \( C_k \) is a constant which is independent of \( \Delta x \) but related to specific candidate stencils.

The weights in Eq. (2.6) are further defined as

\[
\omega_k = \frac{\alpha_k}{\sum_{k=0}^{2} \alpha_k}, \quad \alpha_k = \frac{d_k}{(\beta_k + \epsilon)^q},
\]

where \( d_k \) are optimal weights, i.e.

\[
d_0 = 0.1, \quad d_1 = 0.6, \quad d_2 = 0.3,
\]

which will generate a \((2r-1)\)-th order linear scheme on a \((2r-1)\)-points full stencil, and \( \epsilon \) is a small value that avoids zero denominator. For WENO-JS scheme, the value is given as \( \epsilon = 10^{-6} \). It should be noted that the small value also acts as a cutoff of the smoothness measurement [45], and has been modified to avoid overwhelming small measurements [35]. The nonlinear weights in Eq. (2.11) is the key to suppress the oscillations across discontinuities, and the exponent \( q \geq 1 \) accelerates nonlinear adaptation towards the essentially non-oscillatory property. The exponent is usually defined as \( q = 2 \) for WENO-JS scheme.

The local smoothness indicator \( \beta_k \) in the nonlinear weights determines the contribution of each stencil to the final high order reconstruction, and is defined as

\[
\beta_k = \sum_{j=1}^{2} \Delta x^{2j-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \left( \frac{d}{dx} \hat{f}_k(x) \right)^2 dx.
\]
Jiang and Shu [31] gave the explicit form of the local smoothness indicator in terms of the numerical flux function $f_i$, i.e.

$$
\beta_0 = \frac{1}{4} (f_{i-2} - 4f_{i-1} + 3f_i)^2 + \frac{13}{12} (f_{i-2} - 2f_{i-1} + f_i)^2,
$$

$$
\beta_1 = \frac{1}{4} (f_{i-1} - f_{i+1})^2 + \frac{13}{12} (f_{i-1} - 2f_i + f_{i+1})^2,
$$

$$
\beta_2 = \frac{1}{4} (3f_i - 4f_{i+1} + f_{i+2})^2 + \frac{13}{12} (f_i - 2f_{i+1} + f_{i+2})^2.
$$

(2.14)

### 2.3 WENO-M and WENO-Z schemes

The design of WENO-JS scheme is effective for removing the contribution of the stencil across discontinuity. However, WENO-JS scheme [31] generally degenerates to third-order accuracy near critical points [33], where the first-order derivative vanishes. Since smooth critical points commonly exist in practical simulations, it is expected that the optimal weights in Eq. (2.12) can be achieved in smooth region, or the nonlinear weights can approximately converge to the optimal weights as $\Delta x$ approaches zero.

Henrick et al. [33] investigated the effective order of classical WENO schemes and suggested that satisfying

$$
\sum_{k=0}^{2} (\omega_k - d_k) = O(\Delta x^6),
$$

and

$$
\omega_k - d_k = O(\Delta x^3),
$$

is sufficient for retaining the overall $(2r-1)$-th order accuracy of the nonlinear reconstruction.

Without giving the details of the analysis, the mapping function of Henrick et al. [33] for improving the performance of the weights of fifth-order WENO scheme, can be given as

$$
g_k(\omega) = \frac{\omega(d_k + d_k^2 - 3d_k \omega + \omega^2)}{d_k^2 + \omega(1 - 2d_k)},
$$

and then the weights giving more accurate approximation are calculated by

$$
\alpha_k^* = g_k(\omega_k^{(JS)}).
$$

(2.17)

(2.18)

Eventually, the modified weights are defined according to

$$
\omega_k^{(M)} = \frac{\alpha_k^*}{\sum_{k=0}^{2} \alpha_k^*}, \quad \text{where} \quad \frac{1}{\sum_{k=0}^{2} \alpha_k^*} = 1 + O(\Delta x^3),
$$

and then by using $\omega_k^{(M)}$ instead of the original weights in Eq. (2.6), WENO-M scheme can be given.
Borges et al. [35] suggested that the contribution of the stencil containing discontinuity should be enhanced in the entire reconstruction to improve the accuracy of WENO, without discarding the essentially non-oscillatory property, and further proposed a novel smoothness indicator exploiting the 5 points full stencil of fifth-order schemes, i.e.

$$\tau_5 = |\beta_0 - \beta_2|.$$  

(2.20)

The global smoothness indicator $\tau_5$, is the absolute difference of two local smoothness measures $\beta_0$ and $\beta_2$ and of $O(\Delta x^5)$. It satisfies

$$\frac{\tau_5}{\beta_k + \epsilon} = O(\Delta x^3), \quad k = 1, 2, 3.$$  

(2.21)

Then the new weighting strategy is given as

$$\alpha_{**}^k = d_k \left[1 + \left(\frac{\tau_5}{\beta_k + \epsilon}\right)^q\right],$$  

(2.22)

where $q = 1$ and $\epsilon = 10^{-40}$, and then the final weights $\omega_k^{(Z)}$ of WENO-Z scheme, are calculated by replacing the $\alpha_{**}^k$ in Eq. (2.19) with $\alpha_{**}^k$. It should be noted that, by defining $q = 1$, WENO-Z scheme will be relatively less dissipative comparing with using larger $q$ [35].

By using this weighting strategy, condition Eq. (2.16) is satisfied if there is not critical point. It has been demonstrated that both the weights of WENO-M scheme and WENO-Z scheme converge faster to the optimal weight than that of WENO-JS scheme in smooth solutions. Moreover, the computational cost of WENO-Z scheme is lower than that of WENO-M scheme.

### 2.4 TENO scheme

TENO scheme has been systematically introduced by Fu et al. [42]. Arbitrary high-order spatial accuracy can be attained by the TENO framework which uses a set of low-order stencils with incrementally increasing width. In this section, the simple but effective procedure of fifth-order TENO scheme is introduced.

Inspired by Hu et al. [46] and Borges et al. [35], the smoothness measurement of fifth-order TENO scheme is given as

$$\gamma_k = \left(C + \frac{\tau_5}{\beta_k + \epsilon}\right)^q, \quad k = 0, 1, 2.$$  

(2.23)

It can be found the parameters $\tau_5$ and $\beta_k$ of WENO-JS scheme or WENO-Z scheme have been reused, and the small threshold remains the value of WENO-Z scheme, i.e. $\epsilon = 10^{-40}$. C is set as 1, and the integer power $q$ is set as 6. It should be mentioned that, for fifth-order TENO scheme, the local smooth indicator of WENO-JS scheme, i.e., $\beta_k$, is completely reused. However, for higher order TENO scheme, the incremented-width
stencils are applied, and thus the unified formulation is slightly different with those of classical WENO schemes.

In order to recover the optimal weight in smooth region, TENO scheme does not directly use the weights in Eq. (2.23). The measurement in Eq. (2.23) is normalised at first, i.e.

$$\chi_k = \frac{\gamma_k}{\sum_{k=0}^{2} \gamma_k},$$

(2.24)

and then a cut-off function is defined as

$$\delta_k = \begin{cases} 0, & \text{if } \chi_k < C_T, \\ 1, & \text{otherwise}. \end{cases}$$

(2.25)

Finally, the weights of TENO scheme for Eq. (2.6) are defined by a normalizing procedure

$$\omega_k^{(T)} = \frac{d_k \delta_k}{\sum_{k=0}^{2} d_k \delta_k},$$

(2.26)

where the optimal weights are utilised without rescaling, and only the stencil containing discontinuity is removed from the final reconstruction completely. Therefore, the numerical robustness of TENO scheme can be ensured, and the optimal weight, $d_k$, as well as the accuracy and spectral properties is fully recovered in smooth regions, including at smooth critical points.

It can be found that parameter $C_T$ is also an effective and a direct mean to control the spectral properties of TENO scheme for a specific problem, e.g. compressible turbulence simulation in which embedded shocklets need to be captured without increasing overall dissipation. Haimovich and Frankel [47] has conducted a series of numerical cases, in which the TENO solution with $C_T = 10^{-3}$ is still superior in comparison to the WENO-Z solution. In this paper, the parameter is simply set as $C_T = 10^{-5}$ for all the simulations without detailed discussion.

### 3 Governing equations and solution

For chemical reaction simulations, e.g. denotation, Euler or Navier-Stokes equations with source term need to be solved. Thereinto, detonations of high activation energy mixtures is prone to show irregular cellular structure and highly unstable flow field, for which the turbulence effects should be taken into account [23, 28, 48, 49], and thus Navier-Stokes equations or even large-eddy simulation are necessities for resolving correct flow structures. Since lower numerical viscosity has shown crucial effect on resolving physical viscosity [28], in order to reduce the complexity and investigate the spatial reconstruction specifically, Euler equations are applied and typical test cases affected by physical viscosity insignificantly [5] are used in this work.

Therefore, the methods reconstructing the spatial terms of Euler equations are introduced. Although the complexity of simulating viscous flow is more significant, the
essential ideas of this paper, including the uncoupled method and TENO scheme, can be extended without substantial difficulty. Specifically, the WENO and TENO schemes introduced in the last section will be directly applied for the spatial reconstruction of the presented hyperbolic system, and the captured flow structures are discussed for showing the high resolution property of TENO scheme. Moreover, the extension of TENO scheme is also implemented for implicit large eddy simulation [50], and thus further investigations can be conducted based on the presented results.

3.1 Governing equations

Without loss of generality, the two-dimensional conservative Euler equations involving \( n \) species and reactive source term are written as

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S}. \tag{3.1}
\]

The conservative variables \( \mathbf{U} \), convective fluxes \( \mathbf{F} \) and \( \mathbf{G} \), and reactive source term \( \mathbf{S} \) are

\[
\mathbf{U} = \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho e_t \\
\rho_1 \\
\vdots \\
\rho_{n-1}
\end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
\rho u v \\
\rho (\rho e_t + p) \\
\rho_1 u \\
\vdots \\
\rho_{n-1} u
\end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix}
\rho v \\
\rho u v \\
\rho v^2 + p \\
\rho (\rho e_t + p) \\
\rho_1 v \\
\vdots \\
\rho_{n-1} v
\end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
\sigma_1 \\
\vdots \\
\sigma_{n-1}
\end{pmatrix}, \tag{3.2}
\]

where \( \rho_i \) and \( \sigma_i \) are the density and mass production rate of the \( i \)-th species, which give the total density \( \rho = \sum_{i=1}^{n} \rho_i = \sum_{i=1}^{n} \rho Y_i \) and \( \sum_{i=1}^{n} \sigma_i = 0 \), and \( Y_i \) is the mass fraction of the \( i \)-th species.

The specific heat capacity of the \( i \)-th species at constant pressure is calculated by a polynomial

\[
C_{p,i}(T) = R_i \left( A + BT + C T^2 + D T^3 + E T^4 \right), \tag{3.3}
\]

where \( R_i \) is the gas constant of the \( i \)-th species, and the coefficients of this polynomial is obtained based on the NASA thermochemical polynomial data [51].

The enthalpy of the \( i \)-th species can be written as a function of temperature,

\[
h_i(T) = h_i^T + h_i^0 = \int_{T_{ref}}^{T} C_{p,i}(\tau) d\tau + h_{i,ref}^0, \tag{3.4}
\]

where \( h_i^T \) is the enthalpy associated with temperature, and \( h_{i,ref}^0 \) is the standard enthalpy of formation of the \( i \)-th species. More specifically, there are

\[
h_i^T = \int_{0}^{T} C_{p,i}(\tau) d\tau = R_i \left( A T + \frac{B T^2}{2} + \frac{C T^3}{3} + \frac{D T^4}{4} + \frac{E T^5}{5} \right), \tag{3.5}
\]
and

\[ h_i^0 = h_i^{0,\text{ref}} - \int_0^{T_{\text{ref}}} C_{p,i}(\tau) d\tau. \] (3.6)

The standard enthalpy of formation is given at the specified temperature of \( T_{\text{ref}} = 298 \text{ K} \).

Then the total energy is written as

\[
\rho e_t = \frac{1}{2} \rho (u^2 + v^2) + \rho \sum_{i=1}^{n} Y_i h_i(T) - p. \] (3.7)

It should be noted that the enthalpy in Eq. (3.7) includes the standard enthalpy of formation, which means the energy is related to the mass fraction of components of the gaseous mixture.

### 3.2 The uncoupled formulation

Following the idea of Strang splitting [13], the improvement of uncoupled method [2] further removes \( h_i^{0} \) from the total energy, and thus the equivalent internal energy \( e' \) and enthalpy \( h' \) are defined as

\[
e' = e'_{t} - \frac{1}{2} (u^2 + v^2) = e_t - \sum_{i=1}^{n} Y_i h_i^{0} - \frac{1}{2} (u^2 + v^2), \] (3.8)

and

\[
 h' = h - \sum_{i=1}^{n} Y_i h_i^{0} = \sum_{i=1}^{n} Y_i R_i \left( A T + \frac{B T^2}{2} + \frac{C T^3}{3} + \frac{D T^4}{4} + \frac{E T^5}{5} \right)_i. \] (3.9)

Moreover, the equivalent specific heat ratio \( \gamma' \) can be given following the relation of calorically perfect gas, as

\[
\gamma' = \frac{h'}{e'}. \] (3.10)

Here, \( e' \) and \( \gamma' \) are physically meaningless but makes the energy and specific heat ratio formally equivalent to those forms of calorically perfect gas. Therefore, it will be convenient to extend the perfect gas flow solver for simulating chemical reacting flows.

The modified governing equations are then given as

\[
\frac{\partial \mathbf{U}^*}{\partial t} + \frac{\partial \mathbf{F}^*}{\partial x} + \frac{\partial \mathbf{G}^*}{\partial y} = \mathbf{S}^*, \] (3.11)

where

\[
\mathbf{U}^* = \left( \rho, \rho u, \rho v, \rho e'_t, \rho_1, \ldots, \rho_{n-1} \right)^T, \] (3.12)

\[
\mathbf{S}^* = \left( 0, 0, 0, -\sum_{i=1}^{n} h_i^{0} \cdot \sigma_i, \sigma_1, \ldots, \sigma_{n-1} \right)^T. \] (3.13)
The change of convective fluxes is using the equivalent total energy to replace the original total energy, and then the extra term is added to the right hand side, as a source term.

As aforementioned, Eq. (3.11) is solved by following Strang splitting, i.e. the solutions of flow equation and chemical source term are separated as

\[
\frac{\partial \mathbf{U}^*}{\partial t} + \frac{\partial \mathbf{F}^*}{\partial x} + \frac{\partial \mathbf{G}^*}{\partial y} = 0, \quad (3.14)
\]

\[
\frac{\partial \mathbf{U}^*}{\partial t} = \mathbf{S}^*. \quad (3.15)
\]

The spatial solution method, i.e. TENO scheme in this paper, can be applied for the solution of Eq. (3.14) without modifying the solver of Eq. (3.15).

Strang splitting is applied for attaining second-order temporal accuracy, which is crucial for simulating the unsteady phenomena in this work. Moreover, for the same purpose, Sportisse [52] has further suggested that the last step of the split formulation in each time step should be the stiffness operator, i.e. chemical reaction source term solution in this case, and thus the split sequence is

\[
L(\Delta t) = L_s \left( \frac{\Delta t}{2} \right) L_f(\Delta t) L_s \left( \frac{\Delta t}{2} \right), \quad (3.16)
\]

where the \( L_f \) is the operator of flow equations, Eq. (3.14), and \( L_s \) is the operator of chemical reaction, Eq. (3.15).

The uncoupled method assumes that the total density and the velocity of the gaseous mixture are both constant during the calculation of the source term, which leads to

\[
\frac{\partial \rho}{\partial t} = 0,
\]

\[
\frac{\partial \rho u}{\partial t} = 0,
\]

\[
\frac{\partial \rho v}{\partial t} = 0,
\]

and the density of each species is

\[
\frac{\partial \rho_i}{\partial t} = \sigma_i. \quad (3.18)
\]

The variation of the equivalent total energy is

\[
\frac{\partial \rho e'}{\partial t} = - \sum_{i=1}^{n} h_i^0 \cdot \sigma_i. \quad (3.19)
\]

Because the density and the velocity are both constant in this process, the kinetic energy of the mixture is also constant, i.e.

\[
\frac{\partial}{\partial t} \left[ \frac{\rho(u^2 + v^2)}{2} \right] = 0. \quad (3.20)
\]
Therefore, based on Eqs. (3.18) and (3.19), the energy equation in the chemical reaction process can be written as

\[ \frac{\partial}{\partial t} \left[ \sum_{i=1}^{n} \rho_i \left( h_i + \frac{u^2 + v^2}{2} \right) - p \right] = 0, \quad (3.21) \]

and can be simplified as

\[ \frac{\partial}{\partial t} (\rho h - p) = 0. \quad (3.22) \]

In order to solve the chemical reaction problem, Eqs. (3.18) and (3.22) need to be solved together. These two equations indicate that the reaction process does not change the internal energy of the gaseous mixture, or this reaction is an adiabatic and isovolumetric process. Therefore, aforementioned physical meaningless equivalent energy and equivalent specific heat ratio lead to a physical meaningful formulation.

3.3 Solutions

3.3.1 The solution of flow equations

As aforementioned, the flow equations have been formally transformed to the equations of perfect gas. Therefore, the only modification for solving Eq. (3.14) is replacing the specific heat ratio with the equivalent specific heat ratio. Correspondingly, the modification is implemented for calculating sound speed, as well as the Roe average used for characteristic decomposition and the Global Lax-Friedrichs flux splitting, which are both applied in the numerical computations. Similar strategy has been applied for reacting multi-component flow simulation [53]. As aforementioned, third-order TVD Runge-Kutta scheme is applied for temporal solution, and WENO and TENO can be applied for spatial reconstruction without specific modification.

However, the flow field temperature shall be updated at each time step based on the conservative flow variables which are updated by flow solver directly, for the solution of chemical reaction. After the solution of flow equations, i.e. $\mathcal{L}_f$, the equivalent total energy and the kinetic energy are both given, and thus the equivalent internal energy can be calculated based on Eq. (3.8). The enthalpy is a nonlinear function of temperature, as shown in Eq. (3.9), and thus a formula is given as

\[ e' = \sum_{i=1}^{n} Y_i h_i' - \sum_{i=1}^{n} Y_i R_i T = h' - RT. \quad (3.23) \]

It can be found that Eq. (3.23) is also a nonlinear function of temperature, and then the function can be written as

\[ f(T) = h'(T) - RT - e' = 0. \quad (3.24) \]

$f(T)$ is a monotone increasing function if $T > 0$, and thus it has only one solution. The \textit{zeroin} algorithm [54] is applied to solve this function and to give the temperature.
3.3.2 The solution of chemical reaction

In order to solve the chemical reaction equations, in which temperature is a crucial variable, the reaction equations can be transformed to equations of temperature. For the following equation,

$$\frac{\partial}{\partial t} \left[ \sum_{i=1}^{n} \rho_i (h_i - R_i T) \right] = 0,$$  \hspace{1cm} (3.25)

the differentiation can be given as

$$\sum_{i=1}^{n} \rho_i \frac{\partial}{\partial t} (h_i - R_i T) + \sum_{i=1}^{n} \sigma_i (h_i - R_i T) = 0.$$  \hspace{1cm} (3.26)

Based on

$$\frac{\partial h_i}{\partial t} = \frac{\partial h_i}{\partial T} \frac{\partial T}{\partial t},$$  \hspace{1cm} (3.27)

and Eq. (3.4), one may have

$$\frac{\partial h_i}{\partial t} = C_{P_i}(T) \frac{\partial T}{\partial t}.$$  \hspace{1cm} (3.28)

Substituting Eq. (3.28) into Eq. (3.26), the final formulation is

$$\frac{\partial T}{\partial t} = \frac{\sum_{i=1}^{n} (h_i - R_i T) \sigma_i}{\sum_{i=1}^{n} \rho_i C_{V_i}}.$$  \hspace{1cm} (3.29)

which will be solved by an ODE solver together with Eq. (3.18). In order to deal with the stiffness introduced by the chemical reaction, in which different reactions have different time scales, the prediction-correction-type \(\alpha - QSS\) solver [10] is applied in this paper.

4 Numerical results

Numerical cases are used to verify the performance of the aforementioned schemes. It should be noted that in previous works [42, 43] various test cases involving linear or nonlinear scalar equations, Euler equations and Navier-Stokes equations were solved using TENO scheme. Therefore, in this article, multi-species gaseous flow or reactive flow are considered specifically. However, in order to show an important property of TENO scheme, a 1D linear scalar problem is solved at first.

In the following results, the performance of the schemes for solving the spatial terms is investigated specifically, and third-order Runge-Kutta scheme is used for all the temporal solution. TENO scheme, as aforementioned, attains robustness by completely removing the contribution of those oscillatory stencils, and challenging numerical cases have been introduced [42]. Whereas, some of the WENO schemes improve the accuracy by increasing the contribution of non-smooth stencil, and thus smaller time steps can be necessary for certain extreme test cases. Anyway, robustness is not the primary concern of this article, and thus the time steps for solving the cases of Euler equations are all given based on \(CFL = 0.4\) for consistency and stability.
4.1 One-dimensional linear advection problem

TENO scheme recovers the linear weights for simulating smooth waves, and thus while simulating a smooth field, TENO scheme is expected to behave like a linear scheme in terms of accuracy and resolution, which is the background five-point linear scheme in the presented discussion. A scalar linear advection problem having a smooth field is then applied in this section. The equation to be solved is

\[
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \tag{4.1}
\]

and the initial condition is

\[
u_0(x) = e^{-300(x-x_c)^2}, \quad x_c = 0.5. \tag{4.2}
\]

Periodic boundary condition is used to model the infinite one-dimensional scalar field. The solution at \(t=1\) and between \(x=0\) and \(x=1\), which is one period of the solution, is investigated with using uniformly refined spatial discretization, and the temporal solution time steps are also refined correspondingly to reduce time-integration error.

In Fig. 1, the \(L_1\) and \(L_\infty\) error of WENO-JS scheme, TENO scheme and five-point linear scheme are presented. It is shown that except for coarse discretizations, the resolution and accuracy of TENO scheme are similar to those of the linear scheme. Whereas, WENO-JS scheme is showing lower resolution, although its convergence is also approximately fifth-order. Therefore, it can be concluded that TENO scheme has indeed recovered the background linear scheme in the smooth field, which is due to the improved smoothness measurement and the cut-off procedure.
4.2 Sod shock-tube

Non-reacting multi-species Euler equations are used to test the performance of the presented solver. Here, the Sod shock-tube problem [55] is first applied. In this case, a discontinuity is initially set in the middle of the shock-tube, of which the length is 1, and then the wave structures including shockwave, contact discontinuity and rarefaction wave will evolve along the shock-tube. Moreover, since this work that focuses on reactive flows requires simulating multiple species gas, the non-reacting gaseous mixture of O\textsubscript{2} and N\textsubscript{2} is used to mimic air in the shock tube.

The initial condition is then given as

\[
(\rho, u, p, X_{O_2}, X_{N_2})_{\text{Case A}} = \begin{cases} (1,0,1,0.21,0.79), & \text{if } x \leq 0.5, \\ (0.125,0,1,0.21,0.79), & \text{if } x > 0.5, \end{cases}
\]

\[
(\rho, u, p, X_{O_2}, X_{N_2}, X_{Ar})_{\text{Case B}} = \begin{cases} (1,0,1,0.21,0.79,0), & \text{if } x \leq 0.5, \\ (0.125,0,0.1,0,1), & \text{if } x > 0.5, \end{cases}
\]

where the \(X\) is the fraction of amount of substance. In case A, the mixture mimicking air has filled the shock tube. As aforementioned, the specific heat capacity of each species is calculated by a polynomial interpolation of temperature, and thus the specific heat ratio is the function of temperature as well. The reference temperature in this case is 298K, and it should be noted that changing this parameter will affect the thermodynamic property even in the same non-dimensional initial condition. However, in this case, since N\textsubscript{2} is the major component in the mixture and relatively inert, the gaseous mixture should not be significantly affected by the post shock high temperature. Therefore, it is expected that the numerical result may show agreement with the exact solution of single species calorically perfect gas. On the other hand, in case B, the gaseous mixture is separated with Argon of which the specific heat ratio is 1.66, and thus the preliminary knowledge of wave structures developing across a gas interface can be shown.

In these two cases, 100 equidistant distributed grid points are applied to approximate the one-dimensional shock tube. The numerical results at \(t = 0.2\) is shown. In case A, the exact solution of calorically perfect gas is used as a reference, but in case B, since there is not an exact solution for this problem, the result of WENO-JS scheme calculated on 1000 grid points is used as a reference result.

In Fig. 2, it can be found that WENO schemes and TENO scheme have captured those wave structures, and especially only minor difference can be found in Fig. 2(d). However, TENO scheme has shown superiority, especially near two discontinuities, i.e. shockwave and contact discontinuity. At the meantime, TENO scheme does not introduce any oscillations in the result.

The results of case B are shown in Fig. 3. It is found the interface of difference gases is captured without spurious oscillation. Especially, the travelling shockwave that has crossed the interface of different gas does not cause oscillation. Therefore, the applied method is deemed to be capable for stably capturing shockwaves travelling in non-
Figure 2: The density distribution of case A.

(a) Density along the shock tube

(b) Density near the shockwave

(c) Density near the contact discontinuity

(d) Density near the front of the rarefaction wave

Figure 3: The density distribution of case B.

(a) Density along the shock tube

(b) Specific heat ratio along the shock tube
premixed gas, with using an unified equation of state. The advantage of using TENO scheme can also be found in case B, but the detailed viewing is omitted for simplicity.

### 4.3 Shock-density wave interaction

In order to investigate the performance of the solver in resolving smooth critical points, the classical one-dimensional test case in [56] is applied. In this case, a Mach 3 shockwave travels along the shock-tube, interacting with sine wave in density. This numerical case is especially challenging due to the interaction between shockwave and smooth waves, the accurate simulation of which requires both the numerical dissipation for maintaining stability and the high resolution for resolving smooth critical points. TENO scheme has shown superiority in this case [42,43], but extra features are also taken into account.

As in the last case, non-reacting multi-species gas is also introduced in this case. The computation domain is $[-5,5]$, and discretized by 200 equidistant distributed grid points. Two initial conditions are designed as

\[
\begin{align*}
\text{Case A} &= 
\begin{cases}
(3.8571, 2.6294, 10.3333, 0.21, 0.79), & \text{if } x \leq -4, \\
(1 + 0.2 \sin(5x), 0, 1, 0.21, 0.79), & \text{if } x > -4,
\end{cases} \\
\text{Case B} &= 
\begin{cases}
(3.8571, 2.6294, 10.3333, 0, 1), & \text{if } x \leq -4, \\
(1 + 0.2 \sin(5x), 0, 1, 1, 0), & \text{if } x > -4.
\end{cases}
\end{align*}
\]

Therefore, in case A, the gaseous mixture of $\text{O}_2$ and $\text{N}_2$ mimics air, as in the Sod shock-tube simulation. It is expected that the numerical results of case A are similar with those using single species calorically perfect gas model. On the other hand, in case B, separated $\text{O}_2$ and $\text{N}_2$ fill the shock tube. Both the $\text{O}_2$ and $\text{N}_2$ are diatomic gas, and thus their behavior should be similar with air in moderate temperature. Whereas, with using the reference temperature of 298K, the pure oxygen in case B will be more active in high temperature region which will be produced by the shockwave, and thus the thermodynamic property will be changed more significantly in case B.

Fig. 4 shows the density distributions at $t = 1.8$ of the two cases. The result of WENO-JS scheme with using 2000 grid points is used as the reference result, since there is not a theoretically exact solution. It can be found that TENO scheme shows better resolution in capturing smooth wave structure. WENO-JS scheme with using 200 grid points smears the density wave significantly, which indicates that the numerical dissipation of WENO-JS is significant even in smooth region. WENO-M scheme and WENO-Z scheme show intermediate results between those of WENO-JS and TENO. Therefore, TENO scheme is more accurate than the classical WENO schemes, which is the contribution of recovering the linear weights in the flow field.

In fact, Fig. 4(a) also gives the information about recovering linear scheme in the flow field. The amount of the stencils implemented in each TENO reconstruction is visually shown. It can be found that, in the region of smooth density wave, in general, three candidate stencils are all utilised by TENO, with using the optimal linear weights. Near
the discontinuity, i.e. shockwave, only one stencil is used, to avoid oscillations. In several points of smooth sine wave, one stencil is removed, and in the unperturbed region, many stencils are removed from final reconstructions due to the round-off errors which activate the cut-off procedure of TENO scheme. The similar behaviour can be found in WENO schemes, as well as the second-order finite volume method which uses limiters that are activated in unperturbed flow field [57]. Tuning the $\epsilon$ in Eq. (2.23) can alleviate this phenomenon, but, in general, this numerical behaviour does not affect the accuracy since this region is of constant state.

Furthermore, the results of case A and case B show other information by their difference. In case A, the results are similar with those of the simulations using constant specific heat ratio of $\gamma = 1.4$. On the other hand, in case B, it can be found that the post shock density is higher than that of case A. The reason that causes this difference can be found in Fig. 5, where the specific heat ratio distributions of these two cases are shown.
Figure 5: Specific heat ratio distribution of the shock-density wave interaction problem.

Figure 6: Oxygen density distribution of the shock-density wave interaction problem.

Obviously, in case B, higher mass fraction of O$_2$ in post shock region causes more significant change of the specific heat ratio, because O$_2$ is more sensitive to high temperature, i.e. easier to dissociate. Since the mass fraction of O$_2$ is smaller in post shock region and N$_2$ is relatively inert, the variation of the specific heat ratio is less important in case A. In general, TENO scheme captures the smooth oscillating wave structure more accurately, and the significance of the thermodynamic property of gaseous mixture can be found.

4.4 Steady shock reflection

A steady shockwave reflection problem is simulated to examine the performance of the solver in simulating steady flow. Again, the gaseous mixture of O$_2$ and N$_2$ mimics air. In this case, an oblique shockwave of which the angle is 38.66$^\circ$ is formed in the flow field.
Figure 7: The boundary conditions of the steady shock reflection problem.

The inlet flow Mach number is 2, and the post-shock states are calculated based on the Rankine-Hugoniot conditions. The non-dimensional computation domain is $2 \times 1$, and $100 \times 50$ cells are used for spatial discretization. The boundary conditions are shown in Fig. 7.

WENO-JS, WENO-M, WENO-Z and TENO schemes are all used for simulating this case, and the non-dimensional density contours are shown in Fig. 8. It can be found that TENO scheme captures the sharpest shockwave profile, as in former cases, and there are not spurious oscillations being found. TENO scheme also has advantage in simulating steady multidimensional problems, and more complex simulations are to be shown in the following cases.

Figure 8: Density contours of the steady shock reflection problem. Twenty equally spaced contour lines from $\rho = 1.1$ to $\rho = 1.9$. 
4.5 Shock-bubble interaction

The shock-bubble interaction [58] is simulated to further investigate the solver in simulating non-reacting multi-component flow involving gas interface. In this case, a shockwave will travel along a shock-tube in which an inhomogeneous bubble located in front of the shockwave, and then the shockwave drives the bubble to deform. This case includes abundant shock-interface interaction behaviors including refraction, reflection and scattering, and especially the interface between different density eventually develops to an unstable mixing layer, which can be seemed as RT instability or RM instability with largely distorted initial interface.

In this work, the flow physics is not the primary concern, but the performance of numerical schemes is investigated. WENO-M scheme and TENO scheme are tested in this case. The initial setup in the flow field is shown in Fig. 9. The Mach number of the shockwave located in front of the bubble is 1.22. According to the assumption of Quick and Karni [59], Helium inside the bubble is contaminated by 28% of air, and thus the initial physical property is defined in Table 1. The pressure and density of the gas around the bubble, i.e. region II, are 101325 Pa and 1.225 kg/m³ respectively, and thus the parameters of the gas behind the shockwave, i.e. region III, can be defined based on the shockwave Mach number. The pressure and temperature inside the bubble, i.e. region I, are both equal to those in region II. It should be mentioned that air is mimicked by N₂-O₂ mixture, as in the last two cases. The flow field is discretized by 2000 × 600 equidistant grid points.

![Figure 9: Initial setup of shock-bubble interaction problem.](image)

<table>
<thead>
<tr>
<th>Specific heat ratio</th>
<th>Specific gas constant (kJ/(kg·K))</th>
</tr>
</thead>
<tbody>
<tr>
<td>air</td>
<td>1.4</td>
</tr>
<tr>
<td>28% air + 72% helium</td>
<td>1.648</td>
</tr>
</tbody>
</table>

Numerical results of TENO scheme are shown in Fig. 10. Since Helium/air mixture has larger specific heat ratio, the shockwave in the bubble travels in higher speed compared with the shockwave travelling in the air, which can be clearly found in Fig. 10(a). Due to the higher specific heat ratio and the lower density, the bubble is driven by the
travelling shockwave. It can be found that the interface of the bubble has started to deform, interacting with multiple shockwaves of different scales. In the earlier stage of the simulation, the interface of the bubble has shown insignificant instability, and the difference between the result of each numerical scheme is relatively small.

Whereas, comparison in Fig. 11 indicates that TENO scheme can capture more detailed structures. As aforementioned and shown in Fig. 10, the gas bubble which is of low density and has higher specific heat ratio will be pushed by the heavy and moving
Figure 11: Comparison between TENO scheme and WENO-M scheme.

Air around it, deforming and compressing. Since the velocity of the gas in the bubble is different with that of air, vorticity will drive the interface to form vortex-ring. However, although the shapes of calculated bubbles are similar, TENO scheme captures more clear vortex-ring around the bubble, especially at 380 µs. On the other hand, WENO-M scheme gives barely recognisable vortices in most of the interface. Moreover, the vortex-ring also affects the reflection and scattering of the wave structures around the bubble, which can be visually seemed in the figures, especially in Fig. 11(c). WENO-Z scheme, the results of which are not shown in this case, outperforms WENO-M scheme but is still more dissipa-
tive than TENO scheme. More information will be provided in the following numerical cases.

4.6 Reflection shock induced detonation

The one-dimensional reactive flow phenomenon introduced by Oran et al. [60] is simulated in this case. As described in Fig. 12, a shockwave, of which the Mach number is 2.165, is located in a shock-tube, and travels to the left end of the tube, where solid wall reflects the shockwave, and then the strong reflection ignites the premixed gaseous mixture of H$_2$/O$_2$/Ar. Initially, the ratio of the amount of substance is given as $X_{H_2}:X_{O_2}:X_{Ar} = 2:1:7$, the pressure is 6687Pa, and the temperature is 298K. As shown in Fig. 12, the length of the shock tube is 0.25m.

The experimental result is shown in Fig. 13. The temporal-spatial experimental schlieren of travelling shock-detonation wave shows the complete process of the reflection shock induced detonation. Specifically, four typical incidents are shown in the figure, i.e.

A. Incident shockwave reflects from the left end wall boundary.
B. The gaseous mixture is ignited.
C. The reaction front reaches the reflection shockwave.
D. The rarefaction wave formed at the time of incident C reaches the left end wall boundary.

The experimental result is shown in Fig. 13. The temporal-spatial experimental schlieren of travelling shock-detonation wave shows the complete process of the reflection shock induced detonation. Specifically, four typical incidents are shown in the figure, i.e.

A. Incident shockwave reflects from the left end wall boundary.
B. The gaseous mixture is ignited.
C. The reaction front reaches the reflection shockwave.
D. The rarefaction wave formed at the time of incident C reaches the left end wall boundary.

Figure 12: Initial setup of reflection shock induced detonation.

Figure 13: Time-resolved schlieren photograph of shock reflection-reaction wave formation process [60].
This detailed evolution of the experimental result can be used to examine the capability of reactive flow solver [61], and especially accurately calculating the chemical induction time needs proper numerical scheme and detailed chemistry [34, 62]. In this case, WENO schemes and TENO scheme are tested on 500 and 2000 equidistant grid points, and the 9 species 48 reactions chemical mechanisms of Oran et al. [60] is used for describing the chemical behavior.

In Fig. 14, where the results calculated on 2000 grid points are denoted as fine results, the global maximum pressure is shown to visually find the critical incidents during the evolution of the flow field. The results of WENO-M scheme is similar with those of WENO-JS scheme. and thus they are omitted in the figure for clarity. It can be found that approximately at $t = 13\mu s$, there is a jump of global maximum pressure, which indicates the reflection of the shockwave. About $130\mu s$ later than the reflection, global pressure begins to increase dramatically, which indicates the ignition of the mixture. This result is similar with that of Wu [62]. Specifically, using WENO-JS scheme on sparse discretization gives the earliest ignition, as shown by the blue line in the figure, and grid refinement leads to later ignition in this case. Especially, three schemes on fine grid have presented similar induction times.

Although the induction time is not significantly changed by using different grids and numerical schemes, the maximum pressure during the whole process is varied in different calculations. As shown in Fig. 14, WENO-JS scheme gives lower maximum pressure on 500 grid points. On the other hand, WENO-Z scheme and TENO scheme capture higher maximum pressure on the same sparse grid. Especially, although the variation pattern is somehow different, the maximum pressure peak of TENO scheme on sparse discretization is nearly equal to the fine result. WENO-Z scheme shows high pressure on fine grid, and it is still more sensitive to the grid refinement, comparing with TENO scheme.
Although the experimental result can not show detailed pressure variation, it can be sure that WENO-JS scheme is highly dependent on the grid discretization, probably being caused by its numerical dissipation. Lower pressure could be indicating lower energy release during the simulation. In fact, Oran et al. [5] had investigated the impact of grid resolution, and suggested that sparse mesh can cause inaccurate result in capturing the energy release of detonation phenomena. In this case, TENO scheme and WENO-Z scheme have shown better performance on sparse discretization, and especially TENO scheme captures higher pressure peak on sparse grid.

Some detailed information is given in Fig. 15. In Fig. 15(a), the variation of the pressure distribution indicates that after $210 - 230 \, \mu s$ the peak pressure and the velocity of the detonation wave are stable. In Fig. 15(b), approximately at $t = 193 \, \mu s$, the reaction front reaches the reflected shock wave. Here, only the fine result of TENO scheme is shown, but the general pattern of using the other aforementioned schemes is similar to the presented result. Therefore, the detonation speed can be calculated based on the pressure profile of stabilized travelling detonation wave, and the calculated speed of each simulation is shown in Table 2. The presented results show a little difference comparing with the CJ speed, i.e. $V_{\text{CJ}} = 1616 \, \text{m/s}$, and are nearly equal to the numerical results of Wu et al.

Table 2: Detonation speed (m/s) calculated by different schemes on different grids.

<table>
<thead>
<tr>
<th>Method</th>
<th>500 grid points</th>
<th>2000 grid points</th>
</tr>
</thead>
<tbody>
<tr>
<td>TENO</td>
<td>1674</td>
<td>1673</td>
</tr>
<tr>
<td>WENO-JS</td>
<td>1671</td>
<td>1680</td>
</tr>
<tr>
<td>WENO-M</td>
<td>1673</td>
<td>1687</td>
</tr>
<tr>
<td>WENO-Z</td>
<td>1667</td>
<td>1680</td>
</tr>
</tbody>
</table>
al. [62] and Liu et al. [34]. In general, TENO scheme is capable to describe the ignition and detonation on relative sparse grid.

4.7 Two-dimensional detonation

4.7.1 Computational setup

In this section, the two-dimensional self-sustained detonation which involves interactions between incident shocks, Mach stems, transverse waves, is simulated by using WENO schemes and TENO scheme. It is well known that in the propagating detonation of diluted hydrogen-oxygen mixture, triple points form at the intersection of the transverse wave with the Mach stem and the incident shock, tracing out cellular patterns [63]. This phenomenon is a typical case for testing chemical reaction solver, and simulating the multiple unsteady wave structures is also challenging for both the accuracy and the numerical stability of spatial discretization methods.

In this case, the gaseous mixture is of \( \text{H}_2 / \text{O}_2 / \text{Ar} \), and the ratio of amount of substance is \( X_{\text{H}_2} : X_{\text{O}_2} : X_{\text{Ar}} = 2 : 1 : 7 \). The initial flow field is given by extending the one-dimensional ZND detonation to two-dimensional flow field, in which the traverse velocity \( v \) is zero. Initially, the pressure is 6687\,Pa, and the temperature is 298\,K. Moving coordinate is set on the computational domain, as in [17], which means the inflow velocity and the initial flow velocity are all shifted in the \( x \)-direction by \( -V_{\text{CJ}} \), and thus only the flow field near the detonation front needs to be simulated. In order to attain the self-sustained cellular structure in a short period, an unburnt gas pocket of 10\,mm \( \times \) 14\,mm is located behind the initial detonation front as a physical perturbation [17]. Since the flow field is symmetrical, only upper half of the shock tube is calculated, with using a symmetry boundary condition. It should be noticed that, in reality, the detonation flow field is unsymmetrical, but using a symmetrical half field does not damage the basic behaviour of the detonation phenomenon. Eventually, 0.1\,m \( \times \) 0.03\,m computational domain is given as in Fig. 16.

It has been proved that 700\,\times\,200 grid (Grid A) is sufficient for simulating the self-sustained detonation, with using WENO-M scheme [34]. It is also suggested that one should use 10 cells for discretizing the induction zone [34], the width of which is 1\,mm in this case, and thus 1000\,\times\,300 grid (Grid B) is also applied. The detailed mechanism of Oran et al. [60] is again applied for describing the chemical reaction process.
4.7.2 Basic behavior of the detonation: using TENO scheme

The numerical schlieren calculated by TENO scheme is shown in Fig. 17, in which the original half flow field is mirrored for viewing purposes. In the figures, incident shock, Mach stem, slip line and traverse shock can be found. Specifically, before 50\(\mu s\), there is only one triple point on the half flow field, and the triple point moves from the central line to the wall boundary in Fig. 17(b), being driven by the detonation. Approximately at

Figure 17: Numerical schlieren of two-dimensional detonation: TENO scheme on grid A.
110µs, the second triple point on each half part of the flow field is produced, and then the total four triple points move up and down in the shock tube, of which the pressure peaks are recorded as cellular structure. The cellular structure captured by TENO scheme on Grid A is shown in Fig. 18. The length of the cell is 52mm, and the width is 30mm. The cellular structure calculated on Grid B shows minor difference, and thus it is omitted here.

Several flow field contours at the time near the transition of the triple points, including flow field temperature and one of the intermediate products of the reaction, i.e. HO₂, are shown in Fig. 19. At 100µs, there is still only one triple point on the half flow field, and
then at $110\mu s$, i.e. in Fig. 19(b), the original triple point has started to transit to two triple points. In fact, in Fig. 19(a), there is an unburnt gas pocket can be found behind the Mach stem, according to the lower temperature and the absence of HO$_2$. However, at $110\mu s$, except the original decoupled reaction front, another unburnt gas pocket is formed near the slip line, and the corresponding reaction front eventually develops to the second triple point, as shown in Fig. 19(c). As discussed in [5], weak energy release leads to the decoupled reaction front behind the Mach stem. In other word, the new triple point is formed when the energy release is too low. Therefore, a high resolution scheme can facilitate the detonation simulation since it can capture energy release more accurately, as discussed in the last case. Detailed mechanism of the generation of new triple points is still being investigated and related discussions can be found in various literatures [4, 5, 64, 65], etc..

4.7.3 Comparison

Comparison is made by more results in this section. Firstly, WENO-JS scheme and WENO-M scheme are compared with TENO scheme, and the the numerical schlieren calculated on grid A are shown in Fig. 20. The basic structures in the flow field calculated by each scheme are similar. Thereinto, at $t = 80\mu s$, there is only one triple point on the half flow field, as introduced above. At $t = 150\mu s$, the second triple point in the half flow field can be found, and the underlining mechanism has been briefly introduced. Specifically, TENO scheme has captured more detailed flow structures, including vortices, shear layer and high frequency fluctuations. For example, at $80\mu s$, clear vortices are captured by TENO, behind the slip lines that associate with the Mach stems, but WENO-JS and WENO-M have smeared the vortices significantly, and only a straight slip line is captured by WENO-M. Moreover, at $150\mu s$, TENO scheme captures much more high frequency fluctuations, which probably are caused by larger scale interacting wave structures. For example, the vortices seem to cause abundant small scale travelling fluctuations. WENO-JS scheme also causes a weak inflection on the Mach stem, related to the lower resolution, leading to a new triple point.

WENO-Z has been showing excellent performance in capturing smooth critical points, and it has shown competitive performance in the one-dimensional detonation. Here, the results of WENO-Z and TENO on grid B are shown in Figs. 21-23. Again, TENO scheme has captured much more small scale vortices and fluctuations in the flow field, indicating higher numerical resolution. Thereinto, the slip line associated with triple points have soon developed a series of vortices, yet the vortex structure captured by WENO-Z is relatively weak. Moreover, the bird’s eye views of pressure and temperature have more clearly shown the transverse wave and the vortices in the flow field.

The detonation phenomenon simulated in this section shows regular cellular structure. Lacking of numerical resolution may change the mode number of detonation, i.e. more triple points [5]. On the other hand, further improving the computational resolution does not change the mode number from the correct one, although the shape of the cell can be more precisely described [17]. However, as aforementioned, detonations of high activation energy mixtures is prone to show highly unstable flow field, including
hydrodynamics instabilities, and higher resolution is more important for capturing the correct detonation structures [27].
5 Conclusions

TENO scheme is a novel ENO-like scheme that shows various advantages compared with WENO schemes, as introduced in the original article and the present results. As a novel scheme, there are some aspects of TENO scheme requiring further investigations. For example, the convergence of TENO scheme in simulating steady problems is not yet investigated. Computational convergence could be an issue due to the intrinsic nonlinearity of the scheme, and, in fact, similar problems has also been found in WENO schemes [66] and nonlinear weighted compact schemes [67]. Moreover, it is found that TENO scheme cost 10%–15% more computational time compared with WENO-JS scheme. These issues lead to future works on TENO scheme. However, the advantages of using TENO scheme are still significant.

In this paper, the novel ENO-like scheme, i.e. TENO scheme, is implemented in a reactive flow solver, to simulate various benchmark cases including the two-dimensional
self-sustained detonation phenomenon, with using a simple uncoupled method for splitting the chemical reaction source term. Several one- and two-dimensional numerical cases present new evidences about the high resolution property of TENO scheme, by which complex flow structures can be resolved, even on relatively sparse grids. In fact, the numerical results have indicated that lacking in resolution can potentially lead to essentially incorrect flow structure, due to the highly nonlinearity of detonation phenomena. Moreover, by exploiting the high-resolution property of fifth-order TENO scheme and its improvements, it is also promising to use TENO scheme for simulating reactive flows combining turbulence effects, e.g. turbulence combustion. Especially, the high-resolution property of TENO is attained without the cost of robustness, and thus the flow phenomena containing strong discontinuities, e.g. detonation wave, can be tackled with high fidelity.

Acknowledgments

This work has been financially supported by the National Key Research and Development Program of China (Grant No. 2016YFB0200702) and the National Natural Science Foundation of China (Grant No. 91541117). Dr. Lin Fu has been funded by U.S. Air Force Office of Scientific Research (AFOSR) and Predictive Science Academic Alliance Program (PSAAP).

References


