Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2024-0175

Vol. **39**, No. 5, pp. 1589-1619
May 2026

Stability Analysis and Structure Preserving Schemes for the Reactive Euler Equations with a New Equation of State

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Received 31 July 2024; Accepted (in revised version) 11 February 2025

Abstract. This paper is concerned with the multi-dimensional reactive Euler equations under the new equation of state (EoS) recently proposed in [45]. We show that under this EoS the classical thermodynamic entropy is a strictly convex entropy function in general dimension. Based on this we further prove that the reactive Euler equations satisfy the stability conditions for hyperbolic relaxation systems, which guarantee the existence of zero relaxation limit. The eigen-decompositions of the Jacobian matrices in two and three dimensions are also provided. Moreover, we develop a positivity preserving and oscillation-free entropy stable discontinuous Galerkin scheme by adapting that in [46] for the EoS of ideal gas to the newly proposed one. A key step in doing so is to prove that the HLL (Harten-Lax-van Leer) flux is entropy stable, which is established by tactfully using a natural assumption on a function in the EoS. The high convergence orders stable entropy, no oscillation and positivity of the scheme are demonstrated with numerical examples.

AMS subject classifications: 76M25, 65M60, 65M12

Key words: Reactive Euler equations, strictly convex entropy, stability, entropy stable schemes, discontinuous Galerkin method.

1 Introduction

In this work, we are interested in inviscid compressible reactive Euler equations in D dimensions [9,10]:

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$$\partial_t \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \vdots \\ \rho u_D \\ \rho E \\ \rho Y \end{pmatrix} + \partial_{x_1} \begin{pmatrix} \rho u_1 \\ \rho {u_1}^2 + p \\ \rho u_1 u_2 \\ \vdots \\ \rho u_1 u_D \\ \rho E u_1 + p u_1 \\ \rho u_1 Y \end{pmatrix} + \partial_{x_2} \begin{pmatrix} \rho u_2 \\ \rho u_1 u_2 \\ \rho {u_2}^2 + p \\ \vdots \\ \rho u_2 u_D \\ \rho E u_2 + p u_2 \\ \rho u_2 Y \end{pmatrix} + \cdots + \partial_{x_D} \begin{pmatrix} \rho u_D \\ \rho u_1 u_D \\ \rho u_2 u_D \\ \vdots \\ \rho {u_D}^2 + p \\ \rho E u_D + p u_D \\ \rho u_D Y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \omega \end{pmatrix}, \tag{1.1}$$

where ρ is the fluid density, u_i is the velocity along the direction x_i with $i = 1,2,\cdots,D$, p is the pressure, E is the total energy per unit mass and $Y \in [0,1]$ is the reactant mass fraction. The non-positive source term ω represents the chemical reaction and we adopt the widely used Arrhenius form

$$\omega = -\rho Y \tilde{K} e^{-\tilde{T}/T}, \tag{1.2}$$

where $\tilde{K} > 0$ is a constant rate coefficient, $T = p/\rho$ is the temperature and $\tilde{T} > 0$ is the activation constant temperature. The total energy is related to the internal energy ρe (e is the internal energy per unit mass) as

$$\rho E = \frac{1}{2}\rho \sum_{i=1}^{D} u_i^2 + \rho e + q\rho Y, \tag{1.3}$$

where $q > 0$ is the heat release of reaction. To close the system, we adopt the equation of state (EoS) proposed in [45]:

$$p = (\gamma - 1)(\rho e + q\rho Y - \rho\zeta), \tag{1.4}$$

where γ is the specific heat ratio, $\zeta := \zeta(Y)$ is a smooth function of Y. When $\zeta = 0$, (1.4) degenerates to the EoS for the ideal gas.

For the original Euler equations with chemical reactions of N species, there are N species conservation equations. Unlike this, the reactive Euler equations (1.1) are a simplified system under the assumption that there is only one-step irreversible chemical reaction converting the unreacted species to the reacted species [7,9,10]. Though relatively simple in form, (1.1) can give complicated stable and unstable wave patterns, which have been observed in experiments [2,7]. Due to their practical importance, the reactive Euler equations have been widely investigated both theoretically and numerically in the past decades, see *e.g.* [1,2,4,6,7,11,13,15,16,23,24,35].

Eqs. (1.1) are a system of hyperbolic balance laws and degenerate to the Euler equations when Y = 0. It is well known that hyperbolic balance laws can generate shock discontinuities in a finite time, and thus the solutions are considered in a weak sense and are usually not unique. Then it is necessary to enforce entropy conditions to solve the non-uniqueness problem of weak solutions [8]. In the concept of entropy conditions, there is an entropy function satisfying another conservation (balance) law and it is usually required to be strictly convex [20]. The strict convexity of entropy not only guarantees a unique classical solution to the Cauchy problem of hyperbolic conservation laws, but also induces useful information on the boundary behavior of solutions to initial-boundary-value problems [8, 20].

However, it is recently demonstrated in [44] that for the reactive Euler equations (1.1) with $D=1$ the classical entropy function associated with the thermodynamics is no longer strictly convex under the EoS for the ideal gas. To address this issue two strategies are proposed in [45]. The first one is to correct the entropy function and a class of strictly convex entropy functions are derived by adding an extra term to the classical one. The second strategy is to modify the EoS as (1.4) for the nonideal gas. It is shown in [45] that under certain assumptions of the function ζ the classical entropy function is strictly convex. Additionally, with this EoS the reactive Euler equations are proved to satisfy the stability conditions for general hyperbolic relaxation systems [40], which guarantee the existence of zero relaxation limit. On the other hand, an elegant eigen-system of the Jacobian matrix is presented in [45] and numerical experiments demonstrate that the EoS (1.4) can also generate ZND (Zeldovich-von Neumann-Doering) detonations. Note that these results are established for one dimension.

The aim of this paper is two-fold. First we validate the EoS (1.4) in multi dimensions. We show that for the reactive Euler equations (1.1) in general dimension D, the classical entropy function is still strictly convex under the EoS (1.4). In the multi-dimensional case, the Hessian matrix of the entropy function is quite complicated so that it is difficult to verify its positive definiteness by computing the high order determinants. To address this issue, we adapt the approach in [31] to show that the corresponding quadratic form of the Hessian matrix is positive definite. The proof is not only valid for general dimension but also much simpler than that in [45]. Additionally, we show that the stability conditions in [40] are still admitted in the multi-dimensional case. The eigen-decomposition of the Jacobian matrices of the fluxes are also given explicitly, where the eigenvalues are u_i, u_i+c and u_i-c with c the sound speed.

On the other hand, we develop a positivity preserving and oscillation-free entropy stable discontinuous Galerkin (DG) scheme by adapting that in [46] for the EoS of ideal gas to (1.4). The ingredients of this scheme includes (i) entropy preserving and entropy stable fluxes to achieve entropy stability, (ii) artificial damping terms to restrain spurious oscillations near the shocks, and (iii) positivity preserving limiters to guarantee the positivity of solutions. These ingredients are compatible with each other so that the scheme simultaneously enjoys the properties of entropy stable, oscillation-free and positivity preserving. Here the combination of the first two ingredients is from [26], which merges the entropy stable DG framework [5] and the oscillation-free DG method [25, 27]. The third ingredient, *i.e.*, the positivity limiter, is originally proposed in [42,43]. Based on these, our main task is to specify the entropy preserving and entropy stable fluxes. To this end, we construct entropy preserving flux in the sense of [33] for the reactive Euler equations (1.1) under the EoS (1.4). Additionally, we prove that the HLL (Harten-Lax-van Leer) flux [12] is entropy stable under suitable assumptions on the function ζ in the EoS (1.4). Numerical examples are presented to demonstrate the high order convergence orders and good performance of the scheme for discontinuous problems.

The rest of the paper is organized as follows. In Section 2, we prove that under the EoS (1.4) the classical entropy function is strictly convex. The stability of (1.1) is analysed in Section 3, where the eigen-decompositions of the Jacobian matrices are also provided. In Section 4, we develop a positivity preserving and oscillation-free entropy stable discontinuous Galerkin scheme. Numerical experiments are conducted in Section 5. Finally, some conclusions and remarks are given in Section 6. This paper also has an appendix that gives the eigen-decompositions of the Jacobian matrices in three dimension.

2 Strict convexity of the entropy function

In this section, we show that under the EoS (1.4) the classical entropy function associated with the thermodynamic entropy is strictly convex for the multi-dimensional reactive Euler equations (1.1). Specifically, we denote by $s=\ln(p)-\gamma\ln(\rho)$ the thermodynamic entropy and define

$$\eta=\frac{-\rho s}{\gamma-1},\quad \phi_i=\frac{-\rho s u_i}{\gamma-1},\quad i=1,2,\cdots,D,$$

which are the classical entropy and entropy flux for the Euler equations. It is direct to verify as in [45] that

$$\partial_t\eta+\sum_{i=1}^{D}\partial_{x_i}\phi_i=\frac{\rho}{p}\zeta'\omega. \tag{2.1}$$

Since $\omega\le 0$, the nonpositive entropy production requires that

$$\zeta'(Y)\ge 0,\quad \forall Y\in[0,1]. \tag{2.2}$$

Let $U=(\rho,\rho u_1,\rho u_2,\cdots,\rho u_D,\rho E,\rho Y)^{\dagger}$ with $\dagger$ the transpose operator. We adapt the approach in [31] to show that the quadratic form of the Hessian matrix η_{UU} is positive definite.

Theorem 2.1. *The Hessian matrix η_{UU} is positive definite if and only if $\zeta''>0$, $\forall Y\in[0,1]$.*

Proof. Define $\mu:=\frac{p}{\rho(\gamma-1)}$ and rewrite the thermodynamic entropy as $s=s(\rho,\mu)=\frac{\ln(\gamma-1)}{\gamma-1}+\frac{1}{\gamma-1}\ln\mu-\ln\rho$. Let $T=p/\rho$ be the temperature. It is easy to see that

$$Tds=d\mu+pd\frac{1}{\rho}.$$

With this we denote $\hat{\eta}=(\gamma-1)\eta=-\rho s$ and compute

$$\begin{aligned}\hat{\eta}_U&=-(\rho s_U+se_1)\\&=-\rho(s_\rho e_1+s_\mu\mu_U)-se_1\\&=-\rho s_\mu\mu_U-(\rho s_\rho+s)e_1,\end{aligned}$$

where $e_1=(1,0,0,\cdots,0)\in\mathbb{R}^{D+3}$. Since

$$\begin{aligned}\partial_U(\rho s_\mu\mu_U)&=\rho s_\mu\mu_{UU}+(\rho s_\mu)_U^\dagger\mu_U\\&=\rho s_\mu\mu_{UU}+(s_\mu e_1^\dagger+\rho s_{\mu\rho}e_1^\dagger+\rho s_{\mu\mu}\mu_U^\dagger)\mu_U\\&=\rho s_\mu\mu_{UU}+\rho s_{\mu\mu}\mu_U^\dagger\mu_U+(s_\mu+\rho s_{\mu\rho})e_1^\dagger\mu_U,\\\partial_U[(\rho s_\rho+s)e_1]&=[2s_\rho e_1^\dagger+\rho(s_{\rho\rho}e_1^\dagger+s_{\rho\mu}\mu_U^\dagger)+s_\mu\mu_U^\dagger]e_1\\&=(2s_\rho+\rho s_{\rho\rho})e_1^\dagger e_1+(\rho s_{\rho\mu}+s_\mu)\mu_U^\dagger e_1,\end{aligned}$$

we have

$$\eta_{UU}=-\rho s_\mu\mu_{UU}-\rho s_{\mu\mu}\mu_U^\dagger\mu_U-(s_\mu+\rho s_{\mu\rho})(e_1^\dagger\mu_U+\mu_U^\dagger e_1)-(2s_\rho+\rho s_{\rho\rho})e_1^\dagger e_1.$$

Note that

$$\mu=E-\frac{1}{2}\sum_{i=1}^{D}{u_i}^2-\zeta=\frac{\rho E}{\rho}-\frac{\sum_{i=1}^{D}(\rho u_i)^2}{2\rho^2}-\zeta.$$

We compute

$$\mu_U=\frac{1}{\rho}\left(-\mu+\frac{1}{2}\sum_{i=1}^{D}{u_i}^2+Y\zeta'-\zeta,\quad -u_1,\quad -u_2,\quad \cdots,\quad -u_D,\quad 1,\quad -\zeta'\right)$$

and

$$\mu_{UU}=-\frac{1}{\rho^2}\begin{pmatrix}2(\sum_{i=1}^{D}{u_i}^2-\mu+Y\zeta'-\zeta)+Y^2\zeta'' & -2u_1 & -2u_2 & \cdots & -2u_D & 1 & -\zeta'-Y\zeta''\\ -2u_1 & 1 & 0 & \cdots & 0 & 0 & 0\\ -2u_2 & 0 & 1 & \cdots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots\\ -2u_D & 0 & 0 & \cdots & 1 & 0 & 0\\ 1 & 0 & 0 & \cdots & 0 & 0 & 0\\ -\zeta'-Y\zeta'' & 0 & 0 & \cdots & 0 & 0 & \zeta''\end{pmatrix}.$$

Thus

$$\mu_{UU}+\frac{1}{\rho}(e_1^\dagger\mu_U+\mu_U^\dagger e_1)=-\frac{1}{\rho^2}\begin{pmatrix}\sum_{i=1}^{D}{u_i}^2+Y^2\zeta'' & -u_1 & -u_2 & \cdots & -u_D & 0 & -Y\zeta''\\ -u_1 & 1 & 0 & \cdots & 0 & 0 & 0\\ -u_2 & 0 & 1 & \cdots & 0 & 0 & 0\\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots\\ -u_D & 0 & 0 & \cdots & 1 & 0 & 0\\ 0 & 0 & 0 & \cdots & 0 & 0 & 0\\ -Y\zeta'' & 0 & 0 & \cdots & 0 & 0 & \zeta''\end{pmatrix}.$$

Let $X=(a,b_1,b_2,\cdots,b_D,c,d)^\dagger$ and denote $\alpha=\mu_U X$. We have

$$\begin{aligned}
&X^\dagger\eta_{UU}X\\
=&-\rho s_\mu X^\dagger[\mu_{UU}+\frac{1}{\rho}(e_1^\dagger\mu_U+\mu_U^\dagger e_1)]X-\rho s_{\mu\mu}X^\dagger\mu_U^\dagger\mu_U X\\
&-\rho s_{\mu\rho}X^\dagger(e_1^\dagger\mu_U+\mu_U^\dagger e_1)X-(2s_\rho+\rho s_{\rho\rho})X^\dagger e_1^\dagger e_1 X\\
=&\frac{s_\mu}{\rho}\sum_{i=1}^D(b_i-au_i)^2+\frac{s_\mu}{\rho}\zeta''(d-aY)^2-\rho s_{\mu\mu}\alpha^2-2\rho s_{\mu\rho}a\alpha-(2s_\rho+\rho s_{\rho\rho})a^2.
\end{aligned}$$

Note that

$$s_\mu>0,\quad s_{\mu\mu}<0,\quad s_\rho<0,\quad s_{\rho\rho}<0,\quad \rho^2 s_{\mu\rho}^2<(2s_\rho+\rho s_{\rho\rho})\rho s_{\mu\mu}.$$

Thus η_{UU} is positive definite if and only if $\zeta''>0$. Here we have used the fact that $\sum_{i=1}^D(b_i-au_i)^2+(d-aY)^2+\alpha^2+a^2=0$ if and only if $X=0$. □

Remark 2.1. In one-dimensional case considered in [45], the positive definiteness of the Hessian matrix is proved by showing that all the leading principle minors are positive. However, for the multi-dimensional case, the Hessian matrix is quite complicated so that it is difficult to verify its positive definiteness by computing the high order determinants. Instead, the above proof based on the quadratic form is not only valid for general dimension but also is much simpler than that in [45]. This proof may be applied to many other equations.

Combining (2.1), (2.2) and Theorem 2.1, we have the following conclusion.

Proposition 2.1. The classical entropy function $\eta=\frac{-\rho s}{\gamma-1}$ is a strictly convex entropy for the multi-dimensional reactive Euler equations (1.1) under the EoS (1.4), with ζ satisfying

$$\zeta'(Y)\geq 0,\quad \zeta''(Y)>0,\quad \forall Y\in[0,1]. \tag{2.3}$$

3 Stability and eigen-decomposition of the Jacobian matrix

In this section, we first analyse the stability of the multi-dimensional reactive Euler equations (1.1) under the EoS (1.4) in the sense of hyperbolic relaxation systems [3,37,38,40]. Then we present eigen-decomposition of the Jacobian matrix of the flux. These are extensions of that in [45] for one-dimensional case.

3.1 Stability

For detonation problems, the chemical reaction is very fast so that the rate coefficient $\tilde{K}$ in the reaction term (1.3) is quite large. Thus we introduce a parameter $\epsilon:=1/\tilde{K}$ and write the reactive Euler equation (1.1) as

$$\partial_t U+\sum_{i=1}^D\partial_{x_i}F_i(U)=\frac{1}{\epsilon}Q(U), \tag{3.1}$$

where U takes values in an open subset G of $\mathbb{R}^{D+3}$ and

$$F_i(U)=\left(\rho u_i,\rho u_1 u_i,\cdots,\rho u_{i-1}u_i,\rho u_i{}^2+p,\rho u_{i+1}u_i,\cdots,\rho u_D u_i,\rho E u_i+p u_i,\rho u_i Y\right)^{\dagger},$$
$$Q(U)=(0,0,\cdots,0,-\rho Y e^{-\tilde{T}/T})^{\dagger}.$$

Eqs. (3.1) are a standard hyperbolic system with stiff source term, *i.e.*, hyperbolic relaxation system. For such systems, the following stability conditions are formulated in [40] to guarantee the existence of zero relaxation limit as $\epsilon\to 0$.

(I) There is a strictly convex smooth function $\eta(U)$ such that $\eta_{UU}\partial_U F(U)$ is symmetric for all $U\in G$.

(II) There is a symmetric and non-negative definite matrix $L=L(U)$ such that

$$Q(U)=-L(U)\eta_U(U).$$

(III) The null space of $L(U)$ is independent of $U\in G$.

Here Condition (I) states the existence of a strictly convex entropy function, Condition (II) is an extension of the celebrated Onsager reciprocal relations in nonequilibrium thermodynamics, and Condition (III) expresses the fact that the physical laws of conservation hold true, no matter what state the underlying thermodynamical system is in; see [40] for more details. It is shown in [40] that if a system of PDEs satisfies Conditions (I)-(III), it satisfies all the entropy dissipation conditions in [3,19,28,34,39]. In particular, Conditions (I)-(III) are a strengthened version of the structural stability conditions in [37] for hyperbolic systems of PDEs with relaxation, which guarantee that the solution of the relaxation system converges to that of the equilibrium system in the zero relaxation limit. Moreover, it is observed in [40] that these conditions are satisfied by various models from applications, such as the Euler equations of gas dynamics in vibrational non-equilibrium [41], discrete-ordinate models for radiation hydrodynamics [30], and moment closure systems in kinetic theories [22].

Actually, it has been demonstrated in [36] that Conditions (I)-(III) are not satisfied for the reactive Euler equations under the EoS for the ideal gas. However, for the EoS (1.4), these conditions indeed hold true.

Theorem 3.1. *If ζ satisfies* (2.3) *and $\zeta'(0)=0$, i.e.,*

$$\zeta'(0)=0,\quad \zeta''(Y)>0,\quad \forall Y\in[0,1], \tag{3.2}$$

then the multi-dimensional reactive Euler equations (1.1) *with the EoS* (1.4) *satisfy the stability Conditions (I)-(III).*

Proof. It has been shown in the previous section that $\eta=\frac{-\rho s}{\gamma-1}$ is a strictly convex entropy under the EoS (1.4) with ζ satisfying (2.3). Thus Condition (I) holds and we further check the rest two conditions.

Define a diagonal matrix

$$L(U)=\operatorname{diag}\Big(0,0,0,\cdots,0,0,\frac{Ype^{-\tilde{T}/T}}{\zeta'}\Big)\in\mathbb{R}^{(D+3)\times(D+3)},$$

which satisfies $Q(U)=-L(U)\eta_U(U)$. Note that $\zeta'(0)=0$ and $\zeta''>0$. We get $\zeta'(Y)>0$, $\forall Y\in(0,1]$. When $Y=0$, the numerator and denominator of $\frac{Ype^{-\tilde{T}/T}}{\zeta'}$ are both zero as $\zeta'(0)=0$. Then it follows that

$$\frac{Ype^{-\tilde{T}/T}}{\zeta'}\bigg|_{Y=0}=\frac{pe^{-\tilde{T}/T}}{\zeta''}\bigg|_{Y=0},$$

which is positive since $\zeta''>0$. Thus Condition (II) holds.

Condition (III) is obviously true with the above $L(U)$ and the proof is complete. □

With Conditions (1)-(III) satisfied for the system (3.1) under the EoS (1.4), we can directly apply Theorems 6.1 and 6.2 in [37] to obtain: For smooth initial data, there is a finite and ϵ-independent time interval $[0,\mathcal{T}]$ such that the initial value problem of (3.1) has a unique smooth solution $U^\epsilon=U^\epsilon(t,x)$ defined for $t\in[0,\mathcal{T}]$ and satisfying

$$U^\epsilon=\begin{pmatrix} U^{(eq)} \\ 0 \end{pmatrix}+\mathcal{O}(\epsilon)$$

in a certain Sobolev space, as ϵ goes to zero. Here $U^{(eq)}$ solves the corresponding initial value problem of the equilibrium system of (3.1), *i.e.*, the Euler equations.

3.2 Eigen-system of the Jacobian matrix

In this subsection, we extend the eigen-decomposition of the Jacobian matrix in [45] to the multi-dimensional equations (1.1). The eigen-decomposition, including eigenvalues and eigenvectors, is of practical importance for computations of hyperbolic systems. They are used to formulate the numerical fluxes of many numerical schemes. Here we give the decompositions for two-dimensional case and the three-dimensional results are given in Appendix A.

Consider the two-dimensional reactive Euler equations

$$\partial_t U+\partial_x F(U)+\partial_y G(U)=Q(U), \tag{3.3}$$

where $U=(\rho,\rho u,\rho v,\rho E,\rho Y)^\dagger$, u and v are the fluid velocities along x and y directions, respectively, and

$$\begin{aligned} F(U)&=\big(\rho u,\rho u^2+p,\rho uv,\rho Eu+pu,\rho uY\big)^\dagger,\\ G(U)&=\big(\rho v,\rho uv,\rho v^2+p,\rho Ev+pv,\rho vY\big)^\dagger,\\ Q(U)&=\Big(0,0,0,0,-\rho Y\tilde{K}e^{-\tilde{T}/T}\Big)^\dagger. \end{aligned}$$

With usual notations $H=E+\frac{p}{\rho}$ and $c=\sqrt{\gamma\frac{p}{\rho}}$, we directly compute the Jacobian matrix under the EoS (1.4) as

$$\mathsf{A}=\partial_U F(U)$$
$$=\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -u^2+(\gamma-1)[\frac{1}{2}(u^2+v^2)-(\zeta-\zeta'Y)] & (3-\gamma)u & -(\gamma-1)v & \gamma-1 & -(\gamma-1)\zeta' \\ -uv & v & u & 0 & 0 \\ -Hu+(\gamma-1)[\frac{1}{2}(u^2+v^2)-(\zeta-\zeta'Y)]u & H-(\gamma-1)u^2 & -(\gamma-1)vu & \gamma u & -(\gamma-1)\zeta' u \\ -uY & Y & 0 & 0 & u \end{pmatrix}$$

and

$$\mathsf{B}=\partial_U G(U)$$
$$=\begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ -uv & v & u & 0 & 0 \\ -v^2+(\gamma-1)[\frac{1}{2}(u^2+v^2)-(\zeta-\zeta'Y)] & -(\gamma-1)u & (3-\gamma)v & \gamma-1 & -(\gamma-1)\zeta' \\ -Hv+(\gamma-1)[\frac{1}{2}(u^2+v^2)-(\zeta-\zeta'Y)]v & -(\gamma-1)vu & H-(\gamma-1)v^2 & \gamma v & -(\gamma-1)\zeta' v \\ -vY & 0 & Y & 0 & v \end{pmatrix}.$$

Then we have

Theorem 3.2. *If ζ satisfies* (3.2) *and $\zeta(0)=0$, i.e.,*

$$\zeta(0)=0, \quad \zeta'(0)=0, \quad \zeta''(Y)>0, \quad \forall Y\in[0,1], \tag{3.4}$$

then the Jacobian matrix A *has an eigen-decomposition*

$$\mathsf{A}=\mathsf{R}_\mathsf{A}\, diag(u,u,u,u+c,u-c)\mathsf{L}_\mathsf{A}$$

with

$$\mathsf{R}_\mathsf{A}=\begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ u & 0 & 0 & u+c & u-c \\ v & 0 & 1 & v & v \\ \frac{1}{2}(u^2+v^2) & \zeta' & v & H+uc & H-uc \\ -\frac{\zeta}{\zeta'}+Y & 1 & 0 & Y & Y \end{pmatrix},$$

and

$$
\mathsf{L_A}=\mathsf{R_A}^{-1}
=\begin{pmatrix}
1-\frac{\gamma-1}{2}\frac{u^2+v^2}{c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2} & (\gamma-1)\frac{u}{c^2} & (\gamma-1)\frac{v}{c^2} & -\frac{\gamma-1}{c^2} & \zeta'\frac{\gamma-1}{c^2}\\
-Y+\frac{\zeta}{\zeta'}[1-(\gamma-1)\frac{u^2+v^2}{2c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2}] & (\gamma-1)\frac{\zeta}{\zeta'}\frac{u}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{v}{c^2} & -\frac{\gamma-1}{c^2}\frac{\zeta}{\zeta'} & 1+\zeta\frac{\gamma-1}{c^2}\\
-v & 0 & 1 & 0 & 0\\
\frac{\gamma-1}{4}\frac{u^2+v^2}{c^2}-\frac{1}{2}\frac{u}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2}+\frac{1}{2c} & -\frac{\gamma-1}{2}\frac{v}{c^2} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}\\
\frac{\gamma-1}{4}\frac{u^2+v^2}{c^2}+\frac{1}{2}\frac{u}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2}-\frac{1}{2c} & -\frac{\gamma-1}{2}\frac{v}{c^2} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}
\end{pmatrix}.
$$

And the Jacobian matrix B *also has an eigen-decomposition*

$$
\mathsf{B}=\mathsf{R_B}\,diag(v,v,v,v+c,v-c)\mathsf{L_B}
$$

with

$$
\mathsf{R_B}=\begin{pmatrix}
1 & 0 & 0 & 1 & 1\\
u & 0 & 1 & u & u\\
v & 0 & 0 & v+c & v-c\\
\frac{1}{2}(u^2+v^2) & \zeta' & u & H+vc & H-vc\\
-\frac{\zeta}{\zeta'}+Y & 1 & 0 & Y & Y
\end{pmatrix},
$$

and

$$
\mathsf{L_B}=\mathsf{R_B}^{-1}
=\begin{pmatrix}
1-\frac{\gamma-1}{2}\frac{u^2+v^2}{c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2} & (\gamma-1)\frac{u}{c^2} & (\gamma-1)\frac{v}{c^2} & -\frac{\gamma-1}{c^2} & \zeta'\frac{\gamma-1}{c^2}\\
-Y+\frac{\zeta}{\zeta'}[1-(\gamma-1)\frac{u^2+v^2}{2c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2}] & (\gamma-1)\frac{\zeta}{\zeta'}\frac{u}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{v}{c^2} & -\frac{\gamma-1}{c^2}\frac{\zeta}{\zeta'} & 1+\zeta\frac{\gamma-1}{c^2}\\
-u & 1 & 0 & 0 & 0\\
\frac{\gamma-1}{4}\frac{u^2+v^2}{c^2}-\frac{1}{2}\frac{v}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2} & -\frac{\gamma-1}{2}\frac{v}{c^2}+\frac{1}{2c} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}\\
\frac{\gamma-1}{4}\frac{u^2+v^2}{c^2}+\frac{1}{2}\frac{v}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2} & -\frac{\gamma-1}{2}\frac{v}{c^2}-\frac{1}{2c} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}
\end{pmatrix}.
$$

The proof of the above decompositions is direct and thus is omitted. Here we only point out that $\frac{\zeta}{\zeta'}$ in the decompositions is well defined at $Y=0$ by noting that

$$
\left.\frac{\zeta}{\zeta'}\right|_{Y=0}=\left.\frac{\zeta'}{\zeta''}\right|_{Y=0}=0,
$$

where the condition (3.4) for ζ has been used.

4 Positivity preserving and oscillation-free entropy stable DG scheme

In this section, we develop a positivity preserving and oscillation-free entropy stable DG scheme for the two-dimensional reaction Euler equation (3.3) under EoS (1.4), by adapting that in [46] for the EoS of ideal gas. The main ideal is to combine the oscillation-free entropy stable DG method [5,25–27] and the positivity limiters [42,43]. The scheme thus constructed is entropy stable in the semi-discrete form and is positivity preserving at the full discrete level. Additionally, it can effectively control the spurious oscillations for discontinuous problems.

4.1 SBP matrices and nodal DG scheme

To begin with, we assume the computational domain Ω is periodic or compactly supported, and has a regular partition

$$\Omega = \bigcup_{1\le i\le N_x, 1\le j\le N_y} D_{i,j}, \quad D_{i,j} := I_i \times J_j,$$

where

$$\begin{aligned} I_i &= [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \quad x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots < x_{N_x+\frac{1}{2}}, \quad h_i^x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}, \\ J_j &= [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}], \quad y_{\frac{1}{2}} < y_{\frac{3}{2}} < \cdots < y_{N_y+\frac{1}{2}}, \quad h_j^y = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}. \end{aligned}$$

Additionally, throughout this section we assume numerical solutions are within the admissible state set

$$\mathcal{G} = \{\boldsymbol{u} \in R^5 \,|\, \rho > 0,\ p(\boldsymbol{u}) > 0,\ Y \ge 0\}.$$

This assumption on the positivity is introduced to theoretically prove the entropy stability of the scheme and it can be guaranteed by positivity preserving limiters.

Denote the two-dimensional DG discrete space as

$$V_h^k = \{v_h(x,y) : v_h(x,y)|_{D_{i,j}} \in \Gamma^k(D_{i,j}),\ 1\le i\le N_x,\ 1\le j\le N_y\},$$

where $\Gamma^k(D_{i,j}) = \{\sum_{s,l\le k} c_{s,l} p_s(x) q_l(y) : p_s(x), q_l(y)$ are polynomials of degree $\le k$ with $x\in I_i$ and $y \in J_j\}$. Then our goal is to find a function $U_h \in V_h^k$ such that for any smooth test function $v_h \in V_h^k$

$$\begin{aligned} &\int_{D_{i,j}} (U_h)_t v_h dxdy - \int_{D_{i,j}} F(U_h)\frac{\partial v_h}{\partial x} dxdy - \int_{D_{i,j}} G(U_h)\frac{\partial v_h}{\partial y} dxdy \\ =& -\int_{J_j} [F^x_{i+\frac{1}{2},j} v_h(x^-_{i+\frac{1}{2}}, y_j) - F^x_{i-\frac{1}{2},j} v_h(x^+_{i-\frac{1}{2}}, y_j)] dy \\ & -\int_{I_i} [G^y_{i,j+\frac{1}{2}} v_h(x_i, y^-_{j+\frac{1}{2}}) - G^y_{i,j-\frac{1}{2}} v_h(x_i, y^+_{j-\frac{1}{2}})] dx + \int_{D_{i,j}} Q(U_h) v_h dxdy, \end{aligned} \tag{4.1}$$

where $F^x_{i+\frac{1}{2},j} = \widetilde{F}(U_h(x^-_{i+\frac{1}{2}}, y_j), U_h(x^+_{i+\frac{1}{2}}, y_j))$ and $G^y_{i,j+\frac{1}{2}} = \widetilde{G}(U_h(x_i, y^-_{j+\frac{1}{2}}), U_h(x_i, y^+_{j+\frac{1}{2}}))$ are the numerical fluxes in the x and y directions, respectively.

In order to calculate the integral in the above formula, we introduce the Gauss-Lobato quadrature. Set two-dimensional Gaussian-Lobato orthogonal points as (ξ_r, η_s), $r,s = 0,1,\cdots,m$ on the reference element $R := I \times J = [-1,1]\times[-1,1]$. The corresponding weights are $\omega_r\omega_s$, where ω_r, $r=0,1,\cdots,m$ are the weights in one-dimensional case. Define the two-dimensional Lagrangian node basis functions as

$$L_{rs}(\xi,\eta)=L_r(\xi)L_s(\eta)=\prod_{\substack{l=0\\l\neq r}}^{m}\frac{\xi-\xi_l}{\xi_r-\xi_l}\prod_{\substack{l=0\\l\neq s}}^{m}\frac{\eta-\eta_l}{\eta_s-\eta_l}. \tag{4.2}$$

Using these, we follow [5,21] to define a $(m+1)^2\times(m+1)^2$ matrix

$$L=\left(\vec{L}_{00},\vec{L}_{01},\cdots,\vec{L}_{0m},\vec{L}_{10},\cdots,\vec{L}_{1m},\cdots,\vec{L}_{mm}\right),$$

where

$$\vec{L}_{rs}=(L_{rs}(\xi_0,\eta_0),L_{rs}(\xi_0,\eta_1),\cdots,L_{rs}(\xi_0,\eta_m),L_{rs}(\xi_1,\eta_0),\cdots,L_{rs}(\xi_1,\eta_m),\cdots,L_{rs}(\xi_m,\eta_m))^\dagger.$$

Denote

$$\begin{aligned}L^x&=\left(\partial_x\vec{L}_{00},\partial_x\vec{L}_{01},\cdots,\partial_x\vec{L}_{0m},\partial_x\vec{L}_{10},\cdots,\partial_x\vec{L}_{1m},\cdots,\partial_x\vec{L}_{mm}\right),\\L^y&=\left(\partial_y\vec{L}_{00},\partial_y\vec{L}_{01},\cdots,\partial_y\vec{L}_{0m},\partial_y\vec{L}_{10},\cdots,\partial_x\vec{L}_{1m},\cdots,\partial_y\vec{L}_{mm}\right),\end{aligned}$$

which consist of derivatives of the Lagrangian nodal basis functions with respect to x and y, respectively. Then the two-dimensional discrete difference matrices D^x and D^y can be written as

$$D^xL=L^x,\quad D^yL=L^y.$$

We further introduce the mass matrix

$$M=diag\{\omega_0\omega_0,\omega_0\omega_1,\cdots,\omega_0\omega_m,\omega_1\omega_0,\omega_1\omega_1,\cdots,\omega_1\omega_m,\cdots,\omega_m\omega_m\},$$

the stiffness matrix S^x and S^y

$$S^x:=MD^x,\quad S^y:=MD^y.$$

Then the SBP property gives [5]

$$\begin{aligned}S^x+(S^x)^\dagger=B^x:=&diag\{\tau^x_{00},\tau^x_{01},\cdots,\tau^x_{0m},\tau^x_{10},\cdots,\tau^x_{1m},\cdots,\tau^x_{mm}\}\\=&diag\{-1,0,\cdots,0,1,-1,0,\cdots,0,1,\cdots,-1,0,\cdots,0,1\},\\S^y+(S^y)^\dagger=B^y:=&diag\{\tau^y_{00},\tau^y_{01},\cdots,\tau^y_{0m},\tau^y_{10},\cdots,\tau^y_{1m},\cdots,\tau^y_{mm}\}\\=&diag\{-1,-1,\cdots,-1,0,0,\cdots,0,1,1,\cdots,1\},\end{aligned}$$

where B^x and B^y each have $(m+1)$ 1's and $(m+1)$ -1's.

Denote the r-th diagonal entry of the matrix M as $\hat{\omega}_r$, $r=1,2,\cdots,(m+1)^2$. Similarly, the diagonal entries of B^x and B^y are denoted as $\hat{\tau}_r^x$ and $\hat{\tau}_r^y$, respectively. Then the above matrices enjoy the SBP properties [5,21]:

$$
\begin{aligned}
&(1)\ \ S^x=MD^x, S^y=MD^y,\ \ B^x=S^x+(S^x)^\dagger,\ \ B^y=S^y+(S^y)^\dagger,\\
&(2)\ \ \sum_{l=1}^{(m+1)^2} D_{rl}^x=\sum_{l=1}^{(m+1)^2} D_{rl}^y=0,\quad 1\le r\le (m+1)^2,\\
&(3)\ \ \sum_{l=1}^{(m+1)^2} S_{rl}^x=\sum_{l=1}^{(m+1)^2} \hat{\omega}_r D_{rl}^x=0,\quad 1\le r\le (m+1)^2,\\
&\ \ \sum_{l=1}^{(m+1)^2} S_{rl}^y=\sum_{l=1}^{(m+1)^2} \hat{\omega}_r D_{rl}^y=0,\quad 1\le r\le (m+1)^2,\\
&(4)\ \ \sum_{l=1}^{(m+1)^2} S_{lr}^x=\hat{\tau}_r^x,\ \ \sum_{l=1}^{(m+1)^2} S_{lr}^y=\hat{\tau}_r^y,\quad 1\le r\le (m+1)^2.
\end{aligned}
$$

Using the above SBP properties and the transformations

$$
\begin{aligned}
x_i(\xi_r)&=\frac{1}{2}\left(x_{i-\frac{1}{2}}+x_{i+\frac{1}{2}}\right)+\frac{\xi_r}{2}h_i^x,\\
y_j(\eta_s)&=\frac{1}{2}\left(y_{j-\frac{1}{2}}+y_{j+\frac{1}{2}}\right)+\frac{\eta_s}{2}h_j^y,
\end{aligned}
$$

we can convert (4.1) into [5,21]

$$
\begin{aligned}
&\frac{h_i^x h_j^y}{4}\frac{d\overrightarrow{U^{i,j}}}{dt}+\frac{h_j^y}{2}D^x\overrightarrow{F^{i,j}}+\frac{h_i^x}{2}D^y\overrightarrow{G^{i,j}}\\
=&\frac{h_j^y}{2}M^{-1}B^x(\overrightarrow{F^{i,j}}-\overrightarrow{F_*^{i,j}})+\frac{h_i^x}{2}M^{-1}B^y(\overrightarrow{G^{i,j}}-\overrightarrow{G_*^{i,j}})+\frac{h_i^x h_j^y}{4}\overrightarrow{Q^{i,j}},
\end{aligned}
\tag{4.3}
$$

where

$$
\begin{aligned}
\overrightarrow{U^{i,j}}=&(U_1^{i,j},U_2^{i,j},\cdots,U_{(m+1)^2}^{i,j})^\dagger\\
=&\Big(U(x_i(\xi_0),y_j(\eta_0)),\cdots,U(x_i(\xi_0),y_j(\eta_m)),U(x_i(\xi_1),y_j(\eta_0)),\\
&\cdots,U(x_i(\xi_1),y_j(\eta_m)),\cdots,U(x_i(\xi_m),y_j(\eta_m))\Big)^\dagger,
\end{aligned}
$$

$$
\begin{aligned}
\overrightarrow{F^{i,j}} =& (F_1^{i,j}, F_2^{i,j}, \cdots, F_{(m+1)^2}^{i,j})^\dagger \\
=& \Big(F(x_i(\xi_0), y_j(\eta_0)), \cdots, F(x_i(\xi_0), y_j(\eta_m)), F(x_i(\xi_1), y_j(\eta_0)), \\
& \cdots, F(x_i(\xi_1), y_j(\eta_m)), \cdots, F(x_i(\xi_m), y_j(\eta_m)) \Big)^\dagger, \\
\overrightarrow{G^{i,j}} =& (G_1^{i,j}, G_2^{i,j}, \cdots, G_{(m+1)^2}^{i,j})^\dagger \\
=& \Big(G(x_i(\xi_0), y_j(\eta_0)), \cdots, G(x_i(\xi_0), y_j(\eta_m)), G(x_i(\xi_1), y_j(\eta_0)), \\
& \cdots, G(x_i(\xi_1), y_j(\eta_m)), \cdots, G(x_i(\xi_m), y_j(\eta_m)) \Big)^\dagger, \\
\overrightarrow{Q^{i,j}} =& (Q_1^{i,j}, Q_2^{i,j}, \cdots, Q_{(m+1)^2}^{i,j})^\dagger \\
=& \Big(Q(x_i(\xi_0), y_j(\eta_0)), \cdots, Q(x_i(\xi_0), y_j(\eta_m)), Q(x_i(\xi_1), y_j(\eta_0)), \\
& \cdots, Q(x_i(\xi_1), y_j(\eta_m)), \cdots, Q(x_i(\xi_m), y_j(\eta_m)) \Big)^\dagger,
\end{aligned} \tag{4.4}
$$

and

$$
\begin{aligned}
\overrightarrow{F_*^{i,j}} =& \Big(F(U(x^-_{i-\frac{1}{2}}, y_j(\eta_0)), U(x^+_{i-\frac{1}{2}}, y_j(\eta_0))), 0, \cdots, 0, F(U(x^-_{i+\frac{1}{2}}, y_j(\eta_0)), U(x^+_{i+\frac{1}{2}}, y_j(\eta_0))), \\
& F(U(x^-_{i-\frac{1}{2}}, y_j(\eta_1)), U(x^+_{i-\frac{1}{2}}, y_j(\eta_1))), 0, \cdots, 0, F(U(x^-_{i+\frac{1}{2}}, y_j(\eta_1)), U(x^+_{i+\frac{1}{2}}, y_j(\eta_1))), \\
& F(U(x^-_{i-\frac{1}{2}}, y_j(\eta_m)), U(x^+_{i-\frac{1}{2}}, y_j(\eta_m))), 0, \cdots, 0, F(U(x^-_{i+\frac{1}{2}}, y_j(\eta_m)), U(x^+_{i+\frac{1}{2}}, y_j(\eta_m))) \Big)^\dagger, \\
\overrightarrow{G_*^{i,j}} =& \Big(G(U(x_i(\xi_0), y^-_{j-\frac{1}{2}}), U(x_i(\xi_0), y^+_{j-\frac{1}{2}})), G(U(x_i(\xi_1), y^-_{j-\frac{1}{2}}), U(x_i(\xi_1), y^+_{j-\frac{1}{2}})), \cdots, \\
& G(U(x_i(\xi_m), y^-_{j-\frac{1}{2}}), U(x_i(\xi_m), y^+_{j-\frac{1}{2}})), 0, \cdots, 0, \\
& G(U(x_i(\xi_0), y^-_{j+\frac{1}{2}}), U(x_i(\xi_0), y^+_{j+\frac{1}{2}})), G(U(x_i(\xi_1), y^-_{j+\frac{1}{2}}), U(x_i(\xi_1), y^+_{j+\frac{1}{2}})), \cdots, \\
& G(U(x_i(\xi_m), y^-_{j+\frac{1}{2}}), U(x_i(\xi_m), y^+_{j+\frac{1}{2}})) \Big)^\dagger.
\end{aligned} \tag{4.5}
$$

This is the standard nodal DG scheme for the two-dimensional reactive Euler equations (3.3).

4.2 Entropy stable nodal DG scheme

The node DG scheme (4.3) generally cannot satisfy the entropy stability condition. Here we follow [5] to modify the scheme to be entropy stable under the EoS (1.4). Before that, we introduce the definitions of two-dimensional entropy preserving and entropy stable fluxes in the sense of [33].

Definition 4.1 (entropy preserving flux)**.** Given a entropy function η for (3.3), consistent numerical fluxes $\tilde{F}(U_L,U_R)$ and $\tilde{G}(U_L,U_R)$ are entropy preserving if

$$(V_R-V_L)^\dagger\tilde{F}(U_L,U_R)=\phi_{1,R}-\phi_{1,L},\quad (V_R-V_L)^\dagger\tilde{G}(U_L,U_R)=\phi_{2,R}-\phi_{2,L},$$

where $V_{L,R}$ and $\phi_{i_{L,R}}$ $(i=1,2)$ are the corresponding entropy variables and entropy potential fluxes at the left and right states.

Definition 4.2 (entropy stable flux)**.** Given a entropy function η for (3.3), consistent numerical fluxes $\hat{F}(U_L,U_R)$ and $\hat{G}(U_L,U_R)$ are entropy stable if

$$(V_R-V_L)^\dagger\hat{F}(U_L,U_R)\le\phi_{1,R}-\phi_{1,L},\quad (V_R-V_L)^\dagger\hat{G}(U_L,U_R)\le\phi_{2,R}-\phi_{2,L}.$$

With above definitions, we modify the standard DG scheme (4.3) to be

$$\begin{aligned}&\frac{h_i^x h_j^y}{4}\frac{dU_r^{i,j}}{dt}+h_j^y\sum_{l=1}^{(m+1)^2}D_{rl}^x\tilde{F}(U_r^{i,j},U_l^{i,j})+h_i^x\sum_{l=1}^{(m+1)^2}D_{rl}^y\tilde{G}(U_r^{i,j},U_l^{i,j})\\ =&\frac{h_j^y}{2}\frac{\tau_r^x}{\omega_r}(F_r^{i,j}-F_{*,r}^{i,j})+\frac{h_i^x}{2}\frac{\tau_r^y}{\omega_r}(G_r^{i,j}-G_{*,r}^{i,j})+\frac{h_i^x h_j^y}{4}Q_r^{i,j}\end{aligned}\tag{4.6}$$

with $1\le r\le(m+1)^2$, $1\le i\le N_x$, $1\le j\le N_y$. Here $\tilde{F}$ and $\tilde{G}$ are two-dimensional entropy preserving fluxes and the fluxes in $F_{*,r}^{i,j}$ and $G_{*,r}^{i,j}$ are entropy stable. In this way, the scheme (4.6) is entropy stable for periodic or compactly supported boundary conditions [5].

Next we derive entropy preserving and entropy stable fluxes. Actually, for the reactive Euler equations (3.3) with EoS of the ideal gas, two sets of entropy preserving flux have been proposed in [44]. Here we extend the results to the EoS (1.4). Let a_L and a_R be the values of some variable a at the left and right states, respectively. Denote

$$[\![a]\!]=a_R-a_L,\quad \{\{a\}\}=\frac{1}{2}(a_L+a_R)$$

and introduce the logarithmic average

$$\{\{a\}\}^{\ln}=\frac{[\![a]\!]}{[\![\ln(a)]\!]}.$$

Set a set of algebraic variables

$$z=\begin{pmatrix}z_1\\z_2\\z_3\\z_4\\z_5\end{pmatrix}=\begin{pmatrix}\rho\\u\\v\\\frac{\rho}{p}\\Y\end{pmatrix}.\tag{4.7}$$

Then we propose the following entropy preserving fluxes $\tilde{F}(U_L,U_R):=(\tilde{F}_1,\tilde{F}_2,\cdots,\tilde{F}_5)$ and $\tilde{G}(U_L,U_R):=(\tilde{G}_1,\tilde{G}_2,\cdots,\tilde{G}_5)$:

$$\begin{aligned}
&\tilde{F}_1=\{\{z_1\}\}^{ln}\{\{z_2\}\},\\
&\tilde{F}_2=\{\{z_2\}\}\tilde{F}_1+\frac{\{\{z_1\}\}}{\{\{z_4\}\}},\\
&\tilde{F}_3=\{\{z_3\}\}\tilde{F}_1,\\
&\tilde{F}_4=\Big[\frac{1}{\gamma-1}\frac{1}{\{\{z_4\}\}^{ln}}-\frac{1}{2}(\{\{z_2^2\}\}+\{\{z_3^2\}\})+\{\{\zeta\}\}-\{\{Y\zeta'\}\}\Big]\tilde{F}_1\\
&\qquad+\{\{z_2\}\}\tilde{F}_2+\{\{z_3\}\}\tilde{F}_3+\{\{\zeta'\}\}\tilde{F}_5,\\
&\tilde{F}_5=\Big[-\frac{[\![\zeta]\!]}{[\![\zeta']\!]}+\frac{\{\{\zeta'\}\}[\![z_5]\!]}{[\![\zeta']\!]}+\{\{z_5\}\}\Big]\tilde{F}_1,
\end{aligned}\tag{4.8}$$

and

$$\begin{aligned}
&\tilde{G}_1=\{\{z_1\}\}^{ln}\{\{z_3\}\},\\
&\tilde{G}_2=\{\{z_2\}\}\tilde{G}_1,\\
&\tilde{G}_3=\{\{z_3\}\}\tilde{G}_1+\frac{\{\{z_1\}\}}{\{\{z_4\}\}},\\
&\tilde{G}_4=\Big[\frac{1}{\gamma-1}\frac{1}{\{\{z_4\}\}^{ln}}-\frac{1}{2}(\{\{z_2^2\}\}+\{\{z_3^2\}\})+\{\{\zeta\}\}-\{\{Y\zeta'\}\}\Big]\tilde{G}_1\\
&\qquad+\{\{z_2\}\}\tilde{G}_2+\{\{z_3\}\}\tilde{G}_3+\{\{\zeta'\}\}\tilde{G}_5,\\
&\tilde{G}_5=\Big[-\frac{[\![\zeta]\!]}{[\![\zeta']\!]}+\frac{\{\{\zeta'\}\}[\![z_5]\!]}{[\![\zeta']\!]}+\{\{z_5\}\}\Big]\tilde{G}_1.
\end{aligned}\tag{4.9}$$

Lemma 4.1. *The numerical fluxes* (4.8) *and* (4.9) *are entropy preserving for the entropy* η *under the EoS* (1.4).

Proof. Here we prove that the flux (4.8) is entropy preserving in the sense of Definition 4.1 and the proof for (4.9) is similar. For the entropy $\eta=-\frac{\rho s}{\gamma-1}$ the entropy variable and entropy potential are given by

$$V=\begin{pmatrix}\frac{\gamma-s}{\gamma-1}-\frac{\rho(u^2+v^2)}{2p}+\frac{\rho}{p}(\zeta-\zeta'Y)\\ \rho u/p\\ \rho v/p\\ -\rho/p\\ \rho\zeta'/p\end{pmatrix},\quad \phi_1=\rho u,\quad \phi_2=\rho v.\tag{4.10}$$

Then according to Definition (4.1) we need to prove

$$\Delta_F:=(V_R-V_L)^\intercal\tilde{F}(U_L,U_R)-(\rho u)_R+(\rho u)_L=0.\tag{4.11}$$

We recall from [17] that for the two-dimensional Euler equations without chemical reactions, the entropy variables corresponding to η are

$$V_{Euler}=\begin{pmatrix} \frac{\gamma-s}{\gamma-1}-\frac{\rho(u^2+v^2)}{2p} \\ \rho u/p \\ \rho v/p \\ -\rho/p \end{pmatrix} \tag{4.12}$$

and the entropy preserving (conservative) flux for $F(U)$ is

$$\begin{aligned}\tilde{F}_{Euler}=&\tilde{F}_{Euler}(U_L,U_R)\\ =&\begin{pmatrix} \{\{z_1\}\}^{\ln}\{\{z_2\}\} \\ \frac{\{\{z_1\}\}}{\{\{z_4\}\}}+\{\{z_2\}\}\tilde{F}_1 \\ \{\{z_3\}\}\tilde{F}_1 \\ \left(\frac{1}{(\gamma-1)\{\{z_4\}\}^{\ln}}-\frac{1}{2}\left(\left\{\left\{(z_2)^2\right\}\right\}+\left\{\left\{(z_3)^2\right\}\right\}\right)\right)\tilde{F}_1+\{\{z_2\}\}\tilde{F}_2+\{\{z_3\}\}\tilde{F}_3 \end{pmatrix},\end{aligned} \tag{4.13}$$

where z_i and $\tilde{F}_i(i=1,2,3)$ are the same as (4.7) and (4.8). This indicates that

$$\Delta_{F,Euler}:=(V_{Euler,R}-V_{Euler,L})^{\dagger}\tilde{F}_{Euler}(U_L,U_R)-(\rho u)_R+(\rho u)_L=0. \tag{4.14}$$

Denote the i-th $(i=1,2,3,4)$ component of V_{Euler} and $\tilde{F}_{Euler}$ as $V_{i,Euler}$ and $\tilde{F}_{i,Euler}$, respectively. Then V and $\tilde{F}(U_L,U_R)$ can be written as

$$\begin{aligned} V=&\begin{pmatrix} v_1+\frac{\rho}{p}(\zeta-\zeta' Y) \\ v_2 \\ v_3 \\ v_4 \\ -\zeta' v_4 \end{pmatrix},\\ \tilde{F}(U_L,U_R)=&\begin{pmatrix} \tilde{F}_{1,Euler} \\ \tilde{F}_{2,Euler} \\ \tilde{F}_{3,Euler} \\ \tilde{F}_{4,Euler}+(\{\{\zeta\}\}-\{\{Y\zeta'\}\})\tilde{F}_{1,Euler}+\{\{\zeta'\}\}\tilde{F}_5 \\ \tilde{F}_5 \end{pmatrix}. \end{aligned} \tag{4.15}$$

Combining (4.14) and (4.15), we compute

$$\begin{aligned}
&(V_R-V_L)^\dagger \tilde{F}(U_L,U_R)-(\rho u)_R+(\rho u)_L-\Delta_{F,Euler}\\
=&\left[\!\!\left[\frac{\rho}{p}(\zeta-\zeta' Y)\right]\!\!\right]\tilde{F}_{1,Euler}+[\![v_4]\!]\left((\{\{\zeta\}\}-\{\{Y\zeta'\}\})\tilde{F}_{1,Euler}+\{\{\zeta'\}\}\tilde{F}_5\right)+[\![-\zeta' v_4]\!]\tilde{F}_5\\
=&\left[\!\!\left[\frac{\rho}{p}\zeta\right]\!\!\right]\tilde{F}_{1,Euler}-\left[\!\!\left[\frac{\rho}{p}Y\zeta'\right]\!\!\right]\tilde{F}_{1,Euler}-[\![z_4]\!](\{\{\zeta\}\}-\{\{Y\zeta'\}\})\tilde{F}_{1,Euler}\\
&+\{\{z_4\}\}[\![\zeta']\!]\Big(-\frac{[\![\zeta]\!]}{[\![\zeta']\!]}+\frac{\{\{\zeta'\}\}[\![z_5]\!]}{[\![\zeta']\!]}+\{\{z_5\}\}\Big)\tilde{F}_{1,Euler}\\
=&0.
\end{aligned}$$

This means that (4.8) is entropy preserving and the proof is complete. $\square$

For the entropy stable fluxes $\hat{F}(\cdot,\cdot)$ and $\hat{G}(\cdot,\cdot)$, we take the following two-dimensional HLL (Harten-Lax-van Leer) fluxes [18]:

$$\begin{aligned}
\hat{F}(U_L,U_R)&=\frac{\lambda_R^+F(U_L)-\lambda_L^-F(U_R)+\lambda_R^+\lambda_L^-(U_R-U_L)}{\lambda_R^+-\lambda_L^-},\\
\hat{G}(U_L,U_R)&=\frac{\lambda_R^+G(U_L)-\lambda_L^-G(U_R)+\lambda_R^+\lambda_L^-(U_R-U_L)}{\lambda_R^+-\lambda_L^-},
\end{aligned}\tag{4.16}$$

where $\lambda_L^-=\min(\lambda_L,0)$, $\lambda_R^+=\max(\lambda_R,0)$, and λ_L and λ_R are some approximations of the leftmost wave speed and the rightmost wave speed, respectively. To determine λ_L, λ_R, we first consider the Riemann problem for the Euler equations without chemical reactions and denote $\hat{\lambda}_L$ and $\hat{\lambda}_R$ as the approximations of the leftmost and rightmost wave speed proposed in [5], respectively. Those approximations guarantee that $\hat{\lambda}_L$ is not larger than the true leftmost wave speed and $\hat{\lambda}_R$ is not smaller than the true rightmost wave speed [5]. Then we take λ_L,λ_R such that

$$\lambda_L\le\hat{\lambda}_L<\hat{\lambda}_R\le\lambda_R.\tag{4.17}$$

Lemma 4.2. *Assume λ_L,λ_R satisfy* (4.17) *and ζ satisfies $\zeta''(Y)>0$, $\forall Y\in[0,1]$, then the two-dimensional HLL numerical fluxes* (4.16) *are entropy stable for the entropy η under the EoS* (1.4)*.*

Proof. Here we give the proof for $\hat{F}(U_L,U_R)$ and that for $\hat{G}(U_L,U_R)$ is similar. According to Definition (4.2) we need to prove

$$\Delta_{F,HLL}:=(V_R-V_L)^\dagger\hat{F}(U_L,U_R)-[(\rho u)_R-(\rho u)_L]\le 0.\tag{4.18}$$

Consider the HLL flux for the two-dimensional Euler equations with approximate wave speeds λ_L,λ_R:

$$\begin{aligned}
&\hat{F}_{Euler}(U_{Euler,L},U_{Euler,R})\\
=&\frac{\lambda_R^+F_{Euler}(U_{Euler,L})-\lambda_L^-F_{Euler}(U_{Euler,R})+\lambda_R^+\lambda_L^-(U_{Euler,R}-U_{Euler,L})}{\lambda_R^+-\lambda_L^-}.
\end{aligned}\tag{4.19}$$

Since $\lambda_L \le \hat{\lambda}_L$ and $\lambda_R \ge \hat{\lambda}_R$, according to Corollary 3.2 of [5], the HLL flux (4.19) is entropy stable, *i.e.*,

$$\Delta_{Euler,F,HLL} := (V_{Euler,R} - V_{Euler,L})^\dagger \hat{F}_{Euler}(U_{Euler,L}, U_{Euler,R}) - [(\rho u)_R - (\rho u)_L] \le 0. \tag{4.20}$$

Then we denote $\hat{F}(U_L,U_R) := (\hat{F}_1,\hat{F}_2,\cdots,\hat{F}_5)^\dagger$ and $\hat{F}_{Euler}(U_L,U_R) := (\hat{F}_{1,Euler},\hat{F}_{2,Euler},\hat{F}_{3,Euler},\hat{F}_{4,Euler})^\dagger$ and combine (4.16), (4.19) and (4.20) to compute

$$\begin{aligned}
&\Delta_{F,HLL} - \Delta_{Euler,F,HLL} \\
=& \left[\!\left[\frac{\rho}{p}(\zeta - \zeta' Y) \right]\!\right] \hat{F}_1 + \left[\!\left[-\frac{\rho}{p} \right]\!\right] (\hat{F}_4 - \hat{F}_{4,Euler}) + \left[\!\left[\frac{\rho \zeta'}{p} \right]\!\right] \hat{F}_5 \\
=& \frac{\rho_R \rho_L}{\lambda_R^+ - \lambda_L^-} \lambda_R^+ (\lambda_L^- - u_L)[(Y_R - Y_L)\zeta_R' - (\zeta_R - \zeta_L)] \\
&+ \frac{\rho_R \rho_L}{\lambda_R^+ - \lambda_L^-} \lambda_L^- (u_R - \lambda_R^+)[(Y_R - Y_L)\zeta_L' - (\zeta_R - \zeta_L)].
\end{aligned} \tag{4.21}$$

Note that ζ satisfies $\zeta''(Y) > 0, \forall Y \in [0,1]$, *i.e.*, ζ is a convex function. Then it follows that

$$(Y_R - Y_L)\zeta_R' - (\zeta_R - \zeta_L) \ge 0, \quad (Y_R - Y_L)\zeta_L' - (\zeta_R - \zeta_L) \le 0.$$

On the other hand, since $\hat{\lambda}_L \le u_L$ and $\hat{\lambda}_R \ge u_R$, we have $\lambda_L^- - u_L \le 0$ and $\lambda_R^+ - u_R \ge 0$. Substituting these into (4.21) gives $\Delta_{F,HLL} - \Delta_{Euler,F,HLL} \le 0$ and thereby $\Delta_{F,HLL} \le 0$. This completes the proof. □

Remark 4.1. It is interesting to note that the convexity condition of ζ in Lemma 4.2 is consistent with conditions (3.2) and (3.4). Namely, this condition is required simultaneously for strictly convex entropy, the eigen-decomposition of Jacobian matrices and the entropy stability of the HLL flux. From this point of view, the requirement of convexity on the function ζ is natural.

With the above two lemmas, we have the following theorem, the proof of which is the same as that of Theorems 3.3 and 3.4 in [5].

Theorem 4.1. *Suppose the boundary is periodic or compactly supported. If λ_L,λ_R in the HLL flux* (4.16) *satisfy* (4.17) *and ζ satisfies* (3.4)*, then the scheme* (4.6) *is entropy stable for the entropy η under the EoS* (1.4)*, i.e.,*

$$\frac{d}{dt}\left(\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{r=1}^{(m+1)^2} \frac{h_i^x h_j^y}{4} \hat{\omega}_r \eta(U_r^{i,j}) \right) \le \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{r=1}^{(m+1)^2} \frac{h_i^x h_j^y}{4} \hat{\omega}_r \left(\frac{\rho_r^{i,j}}{p_r^{i,j}} (\zeta')_r^{i,j} \right) Q_r^{i,j}.$$

4.3 Damping terms, positivity preserving limiters and time discretizations

Damping terms and positivity preserving limiters

It is well known that DG schemes usually cause spurious oscillations for problems containing discontinuities. Though the DG scheme (4.6) is entropy stable, it cannot eliminate the spurious oscillation either [5]. To address this issue without destroying the entropy stability, a strategy of adding damping term to the scheme (4.6) is proposed in [26]. This term can not only retain the entropy but also effectively eliminate the spurious oscillations. We add such terms to the scheme (4.6) as in [46] and obtain

$$\begin{aligned}&\frac{h_i^x h_j^y}{4}\frac{dU_r^{i,j}}{dt}+h_j^y\sum_{l=1}^{(m+1)^2}D_{rl}^x\tilde{F}(U_r^{i,j},U_l^{i,j})+h_i^x\sum_{l=1}^{(m+1)^2}D_{rl}^y\tilde{G}(U_r^{i,j},U_l^{i,j})\\ =&\frac{h_j^y}{2}\frac{\tau_r^x}{\omega_r}(F_r^{i,j}-F_{*,r}^{i,j})+\frac{h_i^x}{2}\frac{\tau_r^y}{\omega_r}(G_r^{i,j}-G_{*,r}^{i,j})+\frac{h_i^x h_j^y}{4}Q_r^{i,j}-\sigma_{i,j}(U)\left(U_r^{i,j}-\sum_{k=0}^{(m+1)^2}\frac{\hat{\omega}_k}{4}U_k^{i,j}\right).\end{aligned} \tag{4.22}$$

Here the coefficient $\sigma_{i,j}(U)$ is given by

$$\sigma_{i,j}(U)=\frac{1}{2h_{i,j}}\sum_{l=0}^{1}\left(\max_{1\le s\le 5}\left(\frac{h^{2l}}{(l+1)}\sum_{|\alpha|=l}\Big(\sum_{v\in\partial D_{i,j}}[\![(L\partial^\alpha U)_s|_v]\!]\Big)^2\right)\right)^{\frac{1}{2}}, \tag{4.23}$$

where $h_{i,j}=\sqrt{(h_i^x)^2+(h_j^y)^2}$, $h=\max_{i,j}(h_{i,j})$, and $v\in D_{i,j}$ are the integration points on the boundary $\partial D_{i,j}$. The vector α is the multi-index of order $|\alpha|=\alpha_1+\alpha_2$, $\partial^\alpha\omega=\partial_x^{\alpha_1}\partial_y^{\alpha_2}\omega$, and $(L\partial^\alpha U)_s$ is the s-th component of $L\partial^\alpha U$. The matrix L comes from the characteristic decomposition such that

$$n_1\partial_U F(\bar{U}_{i,j})+n_2\partial_U G(\bar{U}_{i,j})=L^{-1}\Lambda L$$

on the element interface, where $n=(n_1,n_2)$ is the unit out forward normal vector of the element interface and $\bar{U}_{i,j}$ is the arithmetic average at the element interface. Additionally, $[\![\omega]\!]|_v$ denotes the jump of the function ω on the vertex v and we only compute the jump between the element $D_{i,j}$ and its adjacent neighbors. More details can be found in [26]. It is shown in [26] the scheme (4.22) thus obtained is entropy stable and can effectively eliminate the spurious oscillations.

On the other hand, since the average of above damping term in one cell is zero, the scheme (4.22) is compatible with positivity-preserving limiters [26]. Based on this, we impose positivity-preserving limiters to the entropy stable oscillation-free DG scheme (4.22) as in [46]. These limiters guarantee the positivity of the pressure, the density and the mass fraction Y at the fully discrete level. Therefore, the final scheme we obtain is positivity preserving, oscillation-free and entropy stable.

Time discretizations

We further consider the time discretization of the semi-discrete scheme (4.22). For convenience, we write the scheme as

$$\frac{dU}{dt}=\mathbf{S}(U)+\mathbf{N}(U), \tag{4.24}$$

where $\mathbf{S}(U)$ stands for the damping term and $\mathbf{N}(U)$ contains the terms related to the convection part and the source term. Here we consider two kinds of time discretizations. The first kind is the following third-order explicit SSP RK method [32]

$$\begin{aligned} U^{(1)} &= U^n + \Delta t(\mathbf{S}(U^n) + \mathbf{N}(U^n)), \\ U^{(2)} &= \frac{3}{4}U^n + \frac{1}{4}U^{(1)} + \frac{1}{4}\Delta t\left(\mathbf{S}\left(U^{(1)}\right) + \mathbf{N}\left(U^{(1)}\right)\right), \\ U^{n+1} &= \frac{1}{3}U^n + \frac{2}{3}U^{(2)} + \frac{2}{3}\Delta t\mathbf{S}\left(\mathbf{S}\left(U^{(2)}\right) + \mathbf{N}\left(U^{(2)}\right)\right). \end{aligned} \tag{4.25}$$

For some tough problems, the damping term may be quite large, leading to a very restrictive time step for the above method. In this case, we use the following second-order exponential RK method [14]

$$\begin{aligned} U^{(1)} &= e^{-\mu\Delta t}((U^n + \Delta t\mathbf{S}(U^n)) + \Delta t(\mathbf{N}(U^n) + \mu U^n)), \\ U^{n+1} &= \frac{1}{2}e^{-\mu\Delta t}U^n + \frac{1}{2}\left(\left(U^{(1)} + \Delta t\mathbf{S}\left(U^{(1)}\right)\right) + \Delta t\left(\mathbf{N}\left(U^{(1)}\right) + \mu U^{(1)}\right)\right), \end{aligned} \tag{4.26}$$

where μ is a constant.

With the above time discretizations, we refer to [46] and take the time step Δt as

$$\Delta t = \min\left\{ \frac{CFL}{\frac{a_0}{h^x} + \frac{b_0}{h^y}},\quad \frac{\omega_0}{16aa_0}h^x,\quad \frac{\omega_0}{16bb_0}h^y,\quad \frac{1}{2c\tilde{K}}\min_{i,j,r} e^{\tilde{T}/T_r^{i,j}} \right\}, \tag{4.27}$$

where $h^x = \max_i(h_i^x)$, $h^y = \max_j(h_j^y)$, $a_0 = \||u|+c\|_\infty$, $b_0 = \||v|+c\|_\infty$, CFL is CFL number, and $T_r^{i,j,n}$ is the r-th component of the vector $\overrightarrow{T^{i,j}}$. Additionally, a, b and c are proper factors used as approximations to intermediate stages when multiplied by $\||u|+c\|_\infty$ and $\||v|+c\|_\infty$ to ensure the positivity of the SSP RK method. See Remark 4.1 of [46] and Remark 2.7 of [42] for more details. For accuracy test with smooth solutions, we set $\Delta t = \mathcal{O}(\Delta x^{k/m} + \Delta y^{k/m})$ with m the order of the time stepping method and k the degree of DG polynomials.

5 Numerical examples

In this section, we conduct several numerical examples in two dimensions to validate the positivity preserving and oscillation-free entropy stable DG scheme for the reactive Euler equations (3.3) under the EoS (1.4). Unless otherwise stated, the time step is taken as (4.27). According to [11, 42] we take the parameters in the reactive Euler equations as $\gamma = 1.4$, $q = 50$, $\tilde{T} = 50$, $\tilde{K} = 2566.4$. According to conditions (3.2) and (3.4), we take $\zeta = qY^2$ as in [45]. The corresponding EoS is $p = (\gamma-1)[\rho e + q\rho Y(1-Y)]$, which degenerates to the EoS for the ideal gas when $Y = 0,1$.

Example 5.1. We first test convergence orders of the scheme with smooth solutions [46]

$$\rho(x,y,t)=1+0.99\sin(x+y-2t),\quad u=1,\quad v=1,\quad p=1,\quad Y=0$$

in the domain $[0,2\pi]\times[0,2\pi]$. The boundary is periodic and we use P^k elements with $k=2,3,4$. The errors for different mesh sizes at $t=1$ are shown in Table 1, from which designed convergence orders can be observed for k=2,3. While for k=4, the convergence order is one order higher than the designed one.

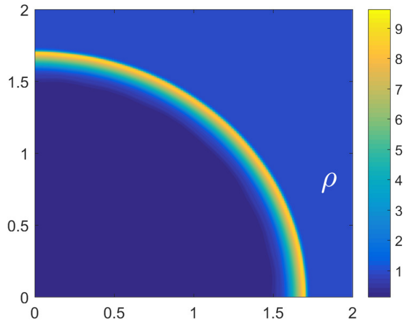
Table 1: Example 5.1: Error table for the problem with smooth solutions. Here $\Delta y=\Delta x$.

			$k=2$			
Δx	l^1 error	order	l^2 error	order	l^∞ error	order
$\pi/4$	3.20e-03		4.80e-03		1.53e-02	
$\pi/8$	7.52e-04	2.09	1.20e-03	2.00	4.3e-03	1.83
$\pi/16$	1.80e-04	2.06	3.25e-04	1.88	1.90e-03	1.18
$\pi/32$	3.14e-05	2.52	6.88e-05	2.24	5.09e-04	1.9
			$k=3$			
Δx	l^1 error	order	l^2 error	order	l^∞ error	order
$\pi/4$	1.10e-03		2.30e-03		8.70e-03	
$\pi/8$	1.57e-04	2.81	5.48e-04	2.07	4.60e-03	0.919
$\pi/16$	1.79e-05	3.13	6.24e-05	3.13	4.93e-04	3.22
$\pi/32$	1.63e-06	3.46	7.05e-06	3.16	8.86e-05	2.48
			$k=4$			
Δx	l^1 error	order	l^2 error	order	l^∞ error	order
$\pi/4$	6.09e-04		1.50e-03		7.90e-03	
$\pi/8$	5.33e-05	3.51	1.61e-04	3.22	1.20e-03	2.72
$\pi/16$	3.34e-06	4.00	1.33e-05	3.6	1.40e-04	3.10
$\pi/32$	8.06e-08	5.37	3.37e-07	5.3	3.89e-06	5.17

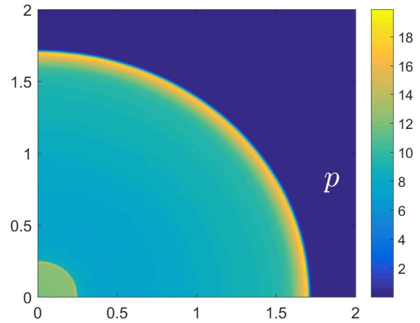
Example 5.2. Next we simulate a two-dimensional explosion wave problem with the following initial condition [35,46]:

$$(\rho,u,v,p,Y)=\begin{cases}(1,0,0,80,0), & x^2+y^2\leqslant 0.36,\\ (1,0,0,10^{-9},1), & x^2+y^2>0.36.\end{cases}$$

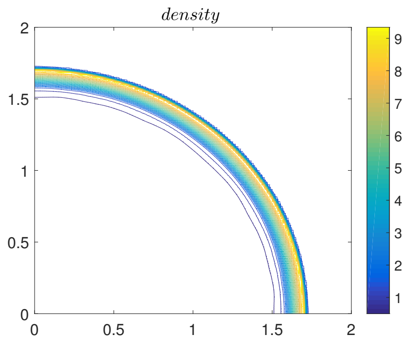
The computational domain is $[0,2]\times[0,2]$ and the left and bottom boundaries are both solid walls. We use the second-order exponential RK method with $CFL=0.5$. Numerical solutions at terminal time $t=0.2$ with $\Delta x=\Delta y=1/60$ are shown in Fig. 1. It can be seen from the figure that we can observe our scheme resolve the structures of blast waves



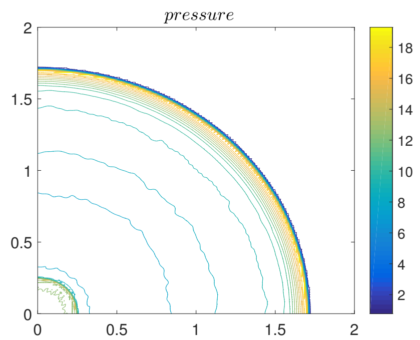
(a) Density



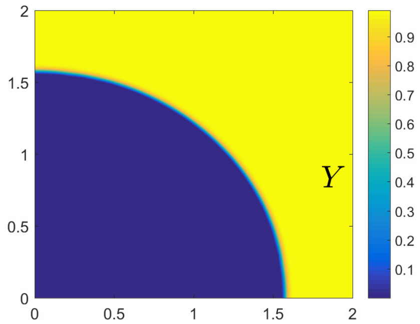
(b) Pressure



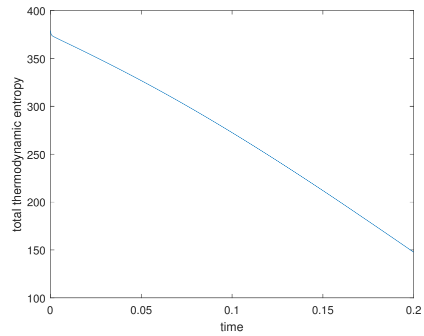
(c) 25 contour lines of density



(d) 25 contour lines of pressure



(e) Mass fraction



(f) Total entropy against time

Figure 1: Example 5.2: Solution profiles at $t=0.2$ and the total entropy against time for the 2D blast wave problem.

successfully without obvious spurious oscillations or entropy increasing. However, there are some slight oscillations for the contour lines of the pressure, even if the mesh is refined as $\Delta x = \Delta y = 1/100$. This may be addressed by adopting a new damping term, *e.g.* the recently proposed one in [29].

Example 5.3. Next we focus on the detonation problem with multiple obstacles. The computational domain is $[0,10]\times[0,8.3]$ and two rectangular obstacles are located in $[1.3,3.3]\times[0,2.6]$ and $[5.1,8.3]\times[0,4.3]$ respectively. The initial condition is

$$(\rho,u,v,p,Y)=\begin{cases}(7,0,0,200,0), & x^2+y^2\leqslant 0.36,\\ (1,0,0,55,1), & x^2+y^2>0.36\end{cases} \tag{5.1}$$

and all the boundaries are solid walls.

To capture small structures near the corners we employ non-uniformly rectangular mesh in Fig. 2. CFL number is taken as 0.65. Solutions at terminal time $t=1$ are plotted in Fig. 3, from which we can see that the complex detonation structures are resolved clearly without oscillations and the total entropy decreases with time. As a comparison, we show in Fig. 4 the pressure and density profiles at the same time $t=1$ under the EoS for the idea gas. It can be observed that the detonation wave transports in a similar way. But the detonation wave under the EoS for the ideal gas has not reached the right obstacle, unlike that under the present one. This indicates that the speed of the detonation wave can be controlled by the new term added in the EoS. It would be interesting to adjust the new term according to the experimental data.

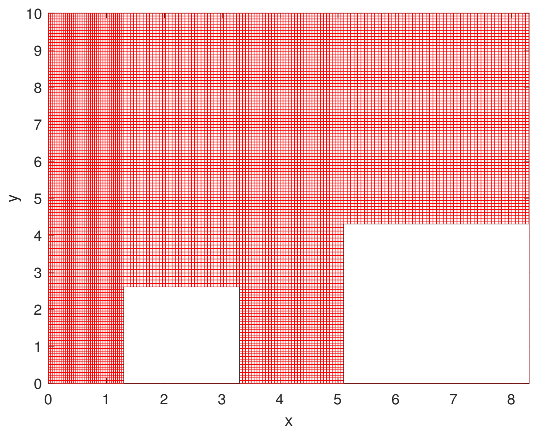
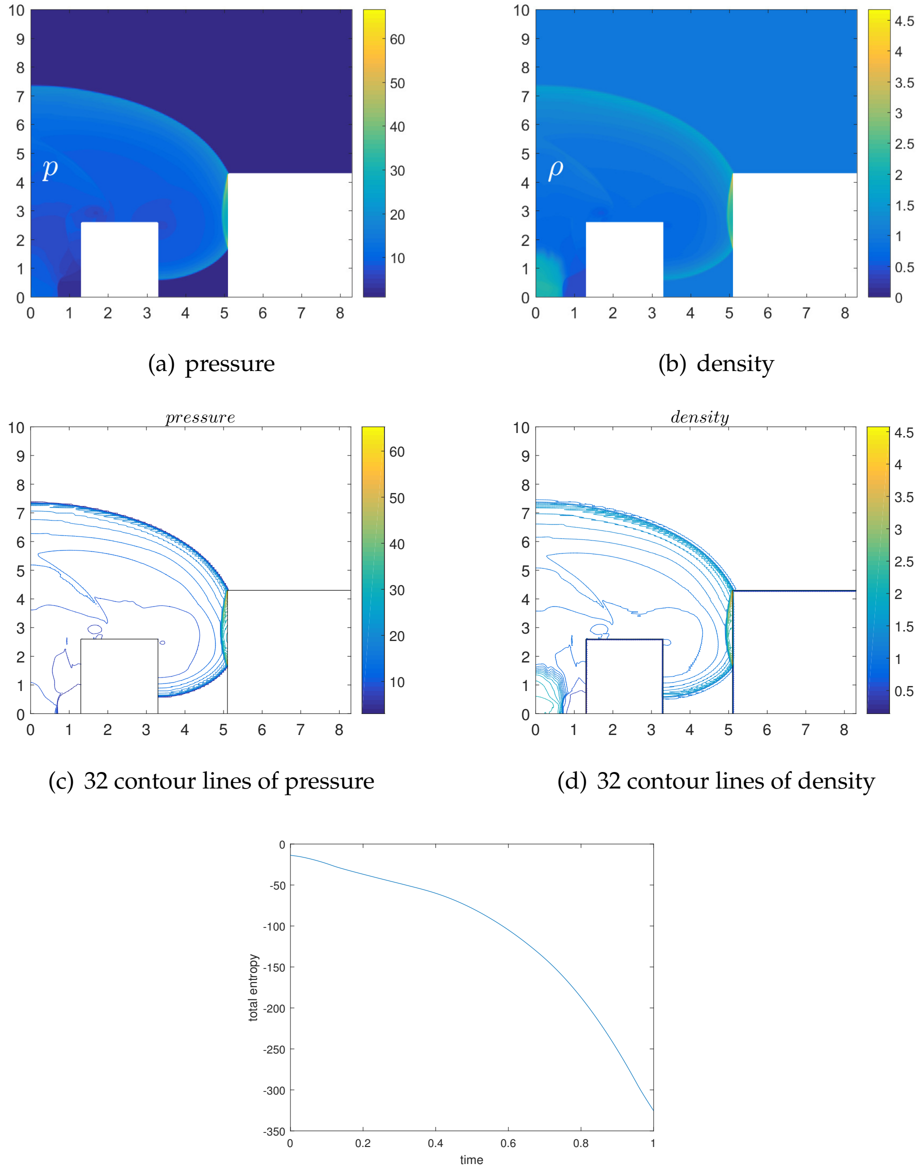


Figure 2: Example 5.3: The non-uniformly rectangular mesh for the detonation problem with multiple obstacles.

6 Conclusions and remarks

In this paper we consider the analysis and computation of multi-dimensional reactive Euler equations under the EoS (1.4). We show that for the reactive Euler equations in general dimension, the classical entropy function is still strictly convex under the EoS (1.4). In this case, the Hessian matrix of the entropy function is quite complicated so that it is difficult



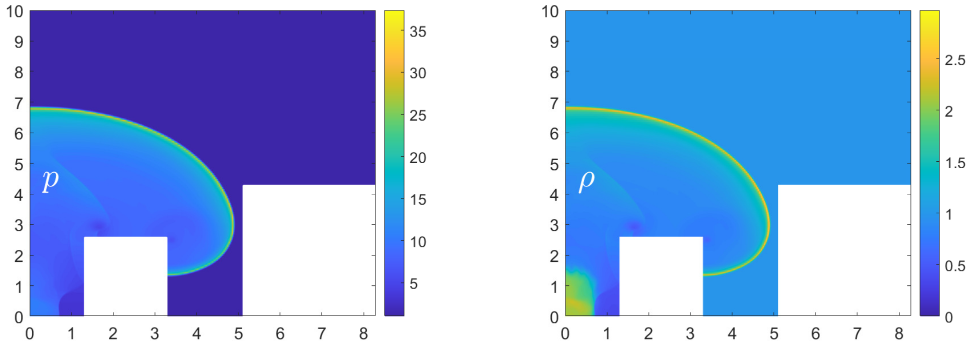
(a) pressure (b) density

(c) 32 contour lines of pressure (d) 32 contour lines of density

(e) Total entropy against time

Figure 3: Example 5.3: Density and pressure profiles at $t=1$ and the total entropy against time for the detonation problem with multiple obstacles.

to verify its positive definiteness by computing the high order determinants. To address this issue, we adapt the approach in [31] to show that the corresponding quadratic form of the Hessian matrix is positive definite. The proof is not only valid for general dimension but also much simpler than that in [45]. Additionally, we show that the stability



(a) pressure (b) density

Figure 4: Example 5.3: Density and pressure profiles at $t=1$ for the detonation problem with multiple obstacles under the EoS for the ideal gas.

conditions in [40] are still admitted in the multi-dimensional case, which guarantee the existence of zero relaxation limit. The eigen-decomposition of the Jacobian matrices of the fluxes are also given explicitly.

On the other hand, we develop a positivity preserving and oscillation-free entropy stable discontinuous Galerkin (DG) scheme by adapting that in [46] for the EoS of ideal gas to (1.4). The ingredients of this scheme includes (i) entropy preserving and entropy stable fluxes to achieve entropy stability, (ii) artificial damping terms to restrain spurious oscillations near the shocks, and (iii) positivity preserving limiters to guarantee the positivity of solutions. These ingredients are compatible with each other so that the scheme simultaneously enjoys the properties of entropy stable, oscillation-free and positivity preserving. To obtain the scheme, we construct entropy preserving flux for the reactive Euler equations under the EoS (1.4). Additionally, we prove that the HLL is entropy stable under suitable assumptions on the function ζ in the EoS (1.4). Numerical examples are presented to demonstrate the high order convergence orders and good performance of the scheme for discontinuous problems.

We would like to point out that the entropy stable scheme we developed here is for rectangular meshes. Extension to triangular meshes can be done as in [5] and is left for our future work. Moreover, since the EoS (1.4) contains a function ζ to be determined, it could be used to fit the solutions of the reactive Euler equations with detailed chemical reactions. In this way, more accurate models are expected to be obtained.

Finally, we remark that for the reactive Euler equations with detailed chemical reactions, the stability conditions (I)-(III) are satisfied under the EoS for the ideal gas [40]. But for the widely used EoS of nonideal gas, there are no such stability results and the wellposedness of the corresponding reactive Euler equations is not clear. Investigation on this interesting topic is left for our future work.

Acknowledgments

Weifeng Zhao would like to thank Prof. Wen-An Yong for helpful discussions on the proof of Theorem 2.1. This work was supported by the National Natural Science Foundation of China (Grant Nos. 12371388 and 12071246) and 2023 Fund for Fostering Young Scholars of the School of Mathematics and Physics, USTB.

Appendix

In this appendix we extend the eigen-decompositions in Subsection 3.2 to three-dimensional reactive Euler equations

$$\partial_t U+\partial_x F(U)+\partial_y G(U)+\partial_z H(U)=Q(U),$$

where

$$\begin{aligned}
&U=(\rho,\rho u,\rho v,\rho w,\rho E,\rho Y)^{\dagger},\\
&F(U)=\left(\rho u,\rho u^2+p,\rho uv,\rho uw,\rho Eu+pu,\rho uY\right)^{\dagger},\\
&G(U)=\left(\rho v,\rho uv,\rho v^2+p,\rho vw,\rho Ev+pv,\rho vY\right)^{\dagger},\\
&H(U)=\left(\rho w,\rho uw,\rho vw,\rho w^2+p,\rho Ew+pw,\rho wY\right)^{\dagger},\\
&Q(U)=(0,0,0,0,0,\omega)^{\dagger}.
\end{aligned}$$

We still define $H=E+\frac{p}{\rho}$ and $c=\sqrt{\gamma\frac{p}{\rho}}$. Then the Jacobian matrices under the EoS (1.4) can be computed as

$$\begin{aligned}
&\mathsf{A}=\partial_U F(U)\\
&=\begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0\\
-u^2+(\gamma-1)[\frac{1}{2}(u^2+v^2+w^2)-(\zeta-\zeta'Y)] & (3-\gamma)u & -(\gamma-1)v & -(\gamma-1)w & \gamma-1 & -(\gamma-1)\zeta'\\
-uv & v & u & 0 & 0 & 0\\
-uw & w & 0 & u & 0 & 0\\
-Hu+(\gamma-1)[\frac{1}{2}(u^2+v^2+w^2)-(\zeta-\zeta'Y)]u & H-(\gamma-1)u^2 & -(\gamma-1)vu & -(\gamma-1)wu & \gamma u & -(\gamma-1)\zeta'u\\
-uY & Y & 0 & 0 & 0 & u
\end{pmatrix},
\end{aligned}$$

$$\begin{aligned}
&\mathsf{B}=\partial_U G(U)\\
&=\begin{pmatrix}
0 & 0 & 1 & 0 & 0 & 0\\
-uv & v & u & 0 & 0 & 0\\
-v^2+(\gamma-1)[\frac{1}{2}(u^2+v^2+w^2)-(\zeta-\zeta'Y)] & -(\gamma-1)u & (3-\gamma)v & -(\gamma-1)w & \gamma-1 & -(\gamma-1)\zeta'\\
-vw & 0 & w & v & 0 & 0\\
-Hv+(\gamma-1)[\frac{1}{2}(u^2+v^2+w^2)-(\zeta-\zeta'Y)]v & -(\gamma-1)vu & H-(\gamma-1)v^2 & -(\gamma-1)vw & \gamma v & -(\gamma-1)\zeta'v\\
-vY & 0 & Y & 0 & 0 & v
\end{pmatrix}
\end{aligned}$$

and

$$
\begin{aligned}
&\mathsf{C}=\partial_U G(U)\\
&=\begin{pmatrix}
0 & 0 & 0 & 1 & 0 & 0\\
-uw & w & 0 & u & 0 & 0\\
-vw & 0 & w & v & 0 & 0\\
-w^2+(\gamma-1)[\frac{1}{2}(u^2+v^2+w^2)-(\zeta-\zeta' Y)] & -(\gamma-1)u & -(\gamma-1)v & (3-\gamma)w & \gamma-1 & -(\gamma-1)\zeta'\\
-Hw+(\gamma-1)[\frac{1}{2}(u^2+v^2+w^2)-(\zeta-\zeta' Y)]w & -(\gamma-1)uw & -(\gamma-1)vw & H-(\gamma-1)w^2 & \gamma w & -(\gamma-1)\zeta' w\\
-wY & 0 & 0 & Y & 0 & w
\end{pmatrix}.
\end{aligned}
$$

The eigen-decompositions of these matrices are given as follows, which can be verified by direct computations.

Theorem A.1. *If ζ satisfies* (3.4), *then the Jacobian matrix* A *has an eigen-decomposition*

$$
\mathsf{A}=\mathsf{R_A}\,diag(u,u,u,u,u+c,u-c)\mathsf{L_A}
$$

with

$$
\mathsf{R_A}=\begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 1\\
u & 0 & 0 & 0 & u+c & u-c\\
v & 0 & 1 & w & v & v\\
w & 0 & 1 & v & w & w\\
\frac{1}{2}(u^2+v^2+w^2) & \zeta' & v+w & 2wv & H+uc & H-uc\\
-\frac{\zeta}{\zeta'}+Y & 1 & 0 & 0 & Y & Y
\end{pmatrix},
$$

and

$$
\begin{aligned}
&\mathsf{L_A}=\mathsf{R_A}^{-1}\\
&=\begin{pmatrix}
1-\frac{\gamma-1}{2}\frac{u^2+v^2+w^2}{c^2}+(\zeta-\zeta' Y)\frac{\gamma-1}{c^2} & (\gamma-1)\frac{u}{c^2} & (\gamma-1)\frac{v}{c^2} & (\gamma-1)\frac{w}{c^2} & -\frac{\gamma-1}{c^2} & \zeta'\frac{\gamma-1}{c^2}\\
-Y+\frac{\zeta}{\zeta'}[1-(\gamma-1)\frac{u^2+v^2+w^2}{2c^2}+(\zeta-\zeta' Y)\frac{\gamma-1}{c^2}] & (\gamma-1)\frac{\zeta}{\zeta'}\frac{u}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{v}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{w}{c^2} & -\frac{\gamma-1}{c^2}\frac{\zeta}{\zeta'} & 1+\zeta\frac{\gamma-1}{c^2}\\
-(w+v) & 0 & \frac{-v}{w-v} & \frac{w}{w-v} & 0 & 0\\
1 & 0 & \frac{1}{w-v} & \frac{-1}{w-v} & 0 & 0\\
\frac{\gamma-1}{4}\frac{u^2+v^2+w^2}{c^2}-\frac{1}{2}\frac{u}{c}-(\zeta-\zeta' Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2}+\frac{1}{2c} & -\frac{\gamma-1}{2}\frac{v}{c^2} & -\frac{\gamma-1}{2}\frac{w}{c^2} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}\\
\frac{\gamma-1}{4}\frac{u^2+v^2+w^2}{c^2}+\frac{1}{2}\frac{u}{c}-(\zeta-\zeta' Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2}-\frac{1}{2c} & -\frac{\gamma-1}{2}\frac{v}{c^2} & -\frac{\gamma-1}{2}\frac{w}{c^2} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}
\end{pmatrix}.
\end{aligned}
$$

The Jacobian matrix B *has an eigen-decomposition*

$$
\mathsf{B}=\mathsf{R_B}\,diag(v,v,v,v+c,v-c)\mathsf{L_B}
$$

with

$$
\mathsf{R_B}=\begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 1\\
u & 0 & 1 & w & u & u\\
v & 0 & 0 & 0 & v+c & v-c\\
w & 0 & 1 & u & w & w\\
\frac{1}{2}(u^2+v^2+w^2) & \zeta' & u+w & 2uw & H+vc & H-vc\\
-\frac{\zeta}{\zeta'}+Y & 1 & 0 & 0 & Y & Y
\end{pmatrix},
$$

and

$$
\mathsf{L_B}=\mathsf{R_B}^{-1}
$$

$$
=\begin{pmatrix}
1-\frac{\gamma-1}{2}\frac{u^2+v^2+w^2}{c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2} & (\gamma-1)\frac{u}{c^2} & (\gamma-1)\frac{v}{c^2} & (\gamma-1)\frac{w}{c^2} & -\frac{\gamma-1}{c^2} & \zeta'\frac{\gamma-1}{c^2}\\
-Y+\frac{\zeta}{\zeta'}[1-(\gamma-1)\frac{u^2+v^2+w^2}{2c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2}] & (\gamma-1)\frac{\zeta}{\zeta'}\frac{u}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{v}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{w}{c^2} & -\frac{\gamma-1}{c^2}\frac{\zeta}{\zeta'} & 1+\zeta\frac{\gamma-1}{c^2}\\
-(u+w) & \frac{-u}{w-u} & 0 & \frac{w}{w-u} & 0 & 0\\
1 & \frac{1}{w-u} & 0 & \frac{-1}{w-u} & 0 & 0\\
\frac{\gamma-1}{4}\frac{u^2+v^2+w^2}{c^2}-\frac{1}{2}\frac{v}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2} & -\frac{\gamma-1}{2}\frac{v}{c^2}+\frac{1}{2c} & -\frac{\gamma-1}{2}\frac{w}{c^2} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}\\
\frac{\gamma-1}{4}\frac{u^2+v^2+w^2}{c^2}+\frac{1}{2}\frac{v}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2} & -\frac{\gamma-1}{2}\frac{v}{c^2}-\frac{1}{2c} & -\frac{\gamma-1}{2}\frac{w}{c^2} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}
\end{pmatrix}.
$$

And the Jacobian matrix C *also has an eigen-decomposition*

$$
\mathsf{C}=\mathsf{R_C}\,diag(w,w,w,w+c,w-c)\mathsf{L_C}
$$

with

$$
\mathsf{R_C}=\begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 1\\
u & 0 & 1 & v & u & u\\
v & 0 & 1 & u & v & v\\
w & 0 & 0 & 0 & w+c & w+c\\
\frac{1}{2}(u^2+v^2+w^2) & \zeta' & u+v & 2uv & H+wc & H-wc\\
-\frac{\zeta}{\zeta'}+Y & 1 & 0 & 0 & Y & Y
\end{pmatrix},
$$

and

$$
\mathsf{L_C}=\mathsf{R_C}^{-1}
$$

$$
=\begin{pmatrix}
1-\frac{\gamma-1}{2}\frac{u^2+v^2+w^2}{c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2} & (\gamma-1)\frac{u}{c^2} & (\gamma-1)\frac{v}{c^2} & (\gamma-1)\frac{w}{c^2} & -\frac{\gamma-1}{c^2} & \zeta'\frac{\gamma-1}{c^2}\\
-Y+\frac{\zeta}{\zeta'}[1-(\gamma-1)\frac{u^2+v^2+w^2}{2c^2}+(\zeta-\zeta'Y)\frac{\gamma-1}{c^2}] & (\gamma-1)\frac{\zeta}{\zeta'}\frac{u}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{v}{c^2} & (\gamma-1)\frac{\zeta}{\zeta'}\frac{w}{c^2} & -\frac{\gamma-1}{c^2}\frac{\zeta}{\zeta'} & 1+\zeta\frac{\gamma-1}{c^2}\\
-(u+v) & \frac{-u}{v-u} & \frac{v}{v-u} & 0 & 0 & 0\\
1 & \frac{1}{v-u} & \frac{-1}{v-u} & 0 & 0 & 0\\
\frac{\gamma-1}{4}\frac{u^2+v^2+w^2}{c^2}-\frac{1}{2}\frac{w}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2} & -\frac{\gamma-1}{2}\frac{v}{c^2} & -\frac{\gamma-1}{2}\frac{w}{c^2}+\frac{1}{2c} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}\\
\frac{\gamma-1}{4}\frac{u^2+v^2+w^2}{c^2}+\frac{1}{2}\frac{w}{c}-(\zeta-\zeta'Y)\frac{\gamma-1}{2c^2} & -\frac{\gamma-1}{2}\frac{u}{c^2} & -\frac{\gamma-1}{2}\frac{v}{c^2} & -\frac{\gamma-1}{2}\frac{w}{c^2}-\frac{1}{2c} & \frac{\gamma-1}{2c^2} & -\zeta'\frac{\gamma-1}{2c^2}
\end{pmatrix}.
$$

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