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Higher Order Accurate Bounds Preserving Time-Implicit Discretizations for the Chemically Reactive Euler Equations

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Abstract. We construct higher order accurate bounds preserving time-implicit Discontinuous Galerkin (DG) discretizations for the reactive Euler equations modelling multispecies and multireaction chemically reactive flows. In numerical discretizations of chemically reactive flows, the time step can be significantly limited because of the large difference between the fluid dynamics time scales and the reaction time scales. In addition, the density and pressure should be nonnegative and the mass fractions between zero and one, which imposes constraints on the numerical solution that must be satisfied to obtain physically reliable solutions. We address these issues using the following steps. Firstly, we develop the Karush-Kuhn-Tucker (KKT) limiter for the chemically reactive Euler equations, which imposes bounds on the numerical solution using Lagrange multipliers, and solve the resulting KKT mixed complementarity problem using a semi-smooth Newton method. The disparity in time scales is addressed using a fractional step method, separating the convection and reaction steps, and the use of higher order accurate Diagonally Implicit Runge-Kutta (DIRK) methods. Finally, Harten's subcell resolution technique is used to deal with stiff source terms in chemically reactive flows. Numerical results are shown to demonstrate that the bounds preserving KKT-DIRK-DG discretizations are higher order accurate for smooth solutions and able to capture complicated stiff multispecies and multireaction flows with discontinuities.

AMS subject classifications: 65M60, 35L60, 35L65, 65M12

Key words: Bounds preserving, DG discretizations, chemically reactive Euler equations, DIRK methods, stiff source terms.

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1 Introduction

Consider the one-dimensional N-species chemically reactive Euler equations [4]

$$U_t+F(U)_x=S(U),\quad (x,t)\in\Omega\times(0,t_T], \tag{1.1}$$

where

$$U=\begin{pmatrix}\rho\\ m\\ E\\ r_1\\ \cdots\\ r_{N-1}\end{pmatrix},\quad F(U)=\begin{pmatrix}m\\ \rho u^2+p\\ (E+p)u\\ \rho u z_1\\ \cdots\\ \rho u z_{N-1}\end{pmatrix},\quad S(U)=\begin{pmatrix}0\\ 0\\ 0\\ s_1\\ \cdots\\ s_{N-1}\end{pmatrix}.$$

Here ρ is the density, u the velocity, $m=\rho u$ the momentum, E the total energy, and z_j $(j=1,\cdots,N)$ the mass fraction of the j-th species with $\sum_{j=1}^N z_j=1$, and $r_j=\rho z_j$. In the following, we compute z_N always using

$$z_N=1-\sum_{j=1}^{N-1} z_j, \tag{1.2}$$

which automatically ensures conservation of species. The pressure is obtained from the equation of state

$$p=\Big(E-\frac{1}{2}\rho u^2-q_1\rho z_1-\cdots-q_N\rho z_N\Big)(\gamma-1), \tag{1.3}$$

where q_j is the enthalpy of formation for the j-th species and γ the ratio of specific heat at constant pressure c_p and constant volume c_v. Physical reliability requires that the density ρ and pressure p are nonnegative and the mass fractions z_j satisfy $z_j\in[0,1]$, $j=1,\cdots,N$. The source terms s_j $(j=1,\cdots,N)$ describe the chemical reactions. For R reactions of the form

$$\nu'_{1,r}X_1+\nu'_{2,r}X_2+\cdots+\nu'_{N,r}X_N\rightarrow\nu''_{1,r}X_1+\nu''_{2,r}X_1+\cdots+\nu''_{N,r}X_N,\quad r=1,\cdots,R,$$

for the species X_j and stoichiometric coefficients $\nu'_{j,r}$ and $\nu''_{j,r}$, the rate of production of species j for the above chemical reaction can be written as

$$s_j=M_j\sum_{r=1}^R(\nu''_{j,r}-\nu'_{j,r})\left[k_r(T)\prod_{k=1}^N\left(\frac{\rho z_k}{M_k}\right)^{\nu'_{k,r}}\right],\quad j=1,2,\cdots,N, \tag{1.4}$$

where M_j denotes the molar mass of the j-th species and $k_r(T)$, which is a function of the temperature $T=\frac{p}{\rho}$ (see [40,41]), indicates the reaction rate. In this paper, we take

$$k_r(T)=\begin{cases}B_rT^{\alpha_r}, & T>T_r,\\ 0, & T\leqslant T_r,\end{cases} \tag{1.5}$$