

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

Fengna Yan<sup>1,2</sup>, J. J. W. Van der Vegt<sup>2</sup>, Yinhua Xia<sup>3</sup> and Yan Xu<sup>3,\*</sup>

<sup>1</sup> School of Mathematical Sciences, Hefei University of Technology, Hefei, Anhui, 230009, P.R. China.

<sup>2</sup> Department of Applied Mathematics, Mathematics of Computational Science Group, University of Twente, Enschede, 7500 AE, The Netherlands.

<sup>3</sup> School of Mathematical Sciences, University of Science and Technology of China, Hefei, Anhui 230026, P.R. China.

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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.

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\*Corresponding author. Email addresses: fnyan@hfut.edu.cn (F. Yan), j.j.w.vandervegt@utwente.nl (J. J. W. Van der Vegt), yhxia@ustc.edu.cn (Y. Xia), yxu@ustc.edu.cn (Y. Xu)

## 1 Introduction

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

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

where

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

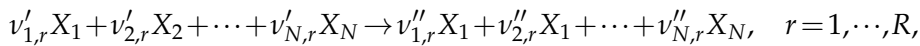
Here  $\rho$  is the density,  $u$  the velocity,  $m = \rho u$  the momentum,  $E$  the total energy, and  $z_j$  ( $j = 1, \dots, N$ ) the mass fraction of the  $j$ -th species with  $\sum_{j=1}^N z_j = 1$ , and  $r_j = \rho z_j$ . In the following, we compute  $z_N$  always using

$$z_N = 1 - \sum_{j=1}^{N-1} z_j, \quad (1.2)$$

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

$$p = \left( E - \frac{1}{2} \rho u^2 - q_1 \rho z_1 - \dots - q_N \rho z_N \right) (\gamma - 1), \quad (1.3)$$

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



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

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

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

$$k_r(T) = \begin{cases} B_r T^{\alpha_r}, & T > T_r, \\ 0, & T \leq T_r, \end{cases} \quad (1.5)$$