Robust and accurate computation of multifluid non-reacting and reacting flows using Discrete Equations Method, anti-diffusive discretization and upwind controlled-downwind splitting

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Abstract: The reactive Riemann solver proposed in [2] is inserted into the Reactive Discrete Equations Method (RDEM) [1, 5] to compute high speed combustion waves. The anti-diffusive approach developed in [4] is also coupled with RDEM to accurately simulate reactive shocks [3]. Increased robustness and efficiency when computing both multiphase interfaces and reacting flows are achieved thanks to an original upwind controlled-downwind splitting method (UCDS).

Keywords: deflagration and denotation, multiphase flows, (Reactive) Discrete Equations Method, anti-diffusive discretization, upwind controlled-downwind splitting

1 Motivation

When numerically investigating multiphase phenomena during severe accidents in a reactor system, characteristic lengths of the multi-fluid zone (non-reactive and reactive) are found to be much smaller than the volume of the reactor containment, which makes the direct modeling of the configuration hardly achievable. Alternatively, we propose to consider the physical multiphase mixture zone as an infinitely thin interface, with specific requirements in the case of reacting flows. For the deflagration case for instance, the fundamental flame speed is imposed so as to make the Riemann problem well-posed. A crucial requirement for this modeling to be of interest is the robust and accurate computation of both impermeable and permeable interfaces.

2 Description of the numerical strategy

The Discrete Equations Method (DEM) initially proposed in [1] for two-phase mixtures and interface problems has been retained as a starting point. The approach has been extended to reactive fronts and christened Reactive DEM (RDEM) in [5] where evaporation fronts were computed. The DEM/RDEM approach considers each fluid has its own pressure, velocity and temperature and relies on the integration of interface problems solutions (derived from sub-cell Riemann problems) over a two-phase control volume. Recently, RDEM has been employed to compute high speed deflagrations and detonations [2]; in order to further enhance the interface capturing, RDEM was also coupled with an anti-diffusive reconstruction proposed in [4] but combustion waves in deflagration regime could not be successfully computed for lack of robustness of the numerical strategy. As illustrated in Fig.1 for a typical Chapman-Jouguet deflagration problem, 1st-order calculations, though possible, yield a very diffused interface which in turn exceedingly moderates the substantial over-pressures physically observed in detonation and fast deflagration. The

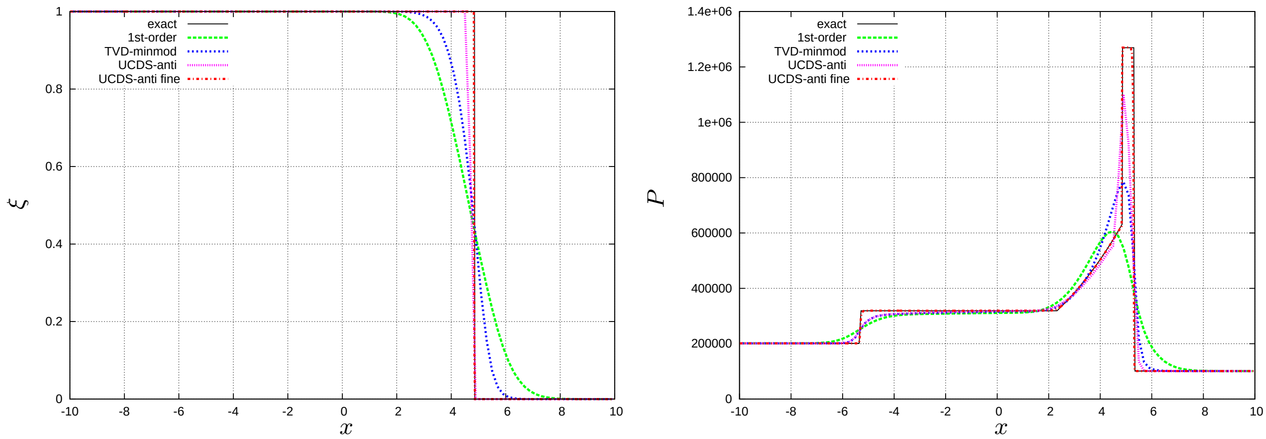

Figure 1: Chapman-Jouguet deflagration : flame reaction rate ξ versus x (left) and pressure P versus x (right) computed with RDEM : 1st-order (100 points), 2nd-order TVD-minmod (100 points) and anti-diffusive UCDS (100/1000 points) discretizations.

present work proposes a simple low-diffusive upwind controlled-downwind splitting (UCDS) for reconstructing the volume fraction within a cell. UCDS provides, in a robust way, very accurate results in the vicinity of the material interface once inserted into DEM or RDEM. As observed in Fig.1, almost exact interface capturing can be achieved using the UCDS idea coupled with an anti-diffusive discretization, which leads to a much better prediction of the pressure distribution for Chapman-Jouguet deflagration. Note also UCDS increases the robustness of RDEM coupled with a second-order MUSCL approach using a minmod limiter (without UCDS the calculation can fail). The numerical strategy combining DEM/RDEM with an anti-diffusive discretization and UCDS was found more robust and accurate than the original MUSCL-based DEM developed in [1] as well as the original anti-diffusive approach [4] coupled with DEM/RDEM, for a wide range of both reactive and non-reactive flows (such as two-phases flows of fluids governed by stiffened-gas equation of states). Higher computational efficiency is also achieved because the steeper representation of the interface reduces the zone where expensive reactive Riemann problems have to be computed within RDEM. 1D and multi-D results obtained through the implementation of the approach within the general-purpose Europlexus code will be presented at the Conference.

References

[1] R Abgrall and R Saurel. Discrete equations for physical and numerical compressible multiphase mixtures. *J. Comput. Phys.*, 186(2):361–396, 2003.

[2] A Beccantini and E Studer. The reactive Riemann problem for thermally perfect gases at all combustion regimes. *Int. J. Numer. Meth. Fluids*, 64:269–313, 2010.

[3] A Beccantini and K Tang. The Reactive Discrete Equations Method for the (reactive) Euler Equations: the minmod reconstruction versus the antidiffusive approach. Technical report, CEA Saclay DM2S/SFME/LTMF/RT/10-007/A, 2010.

[4] B Després and F Lagoutière. Contact Discontinuity Capturing Schemes for Linear Advection and Compressible Gas Dynamics. *J. of Scientific Computing*, 16(4):479–524, 2002.

[5] O Lemetayer, J Massoni, and R Saurel. Modelling evaporation fronts with reactive Riemann solvers. *J. Comput. Phys.*, 205(2):567–610, 2005.