

Fully-Implicit Density-Based Algorithms for Simulations of Arbitrary Gas Mixtures

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Abstract

A robust and straightforward extension of Roe’s approximate Riemann solver to chemically reacting flows is presented in this paper. Flux-difference-splitting and flux-splitting methods for general, reacting gas mixtures are obtained via a formulation based on the excess internal energy of the mixture with respect to its ideal, thermally perfect gas state. A practical, fully implicit algorithm is derived. Detailed derivations of the Roe-average state, as well as of the transformation Jacobians are shown for the case of a reacting mixture of ideal gas species with variable specific heats. The algorithm is suitable for models with detailed thermochemistry as well as reduced models, e.g. based on progress variables. Results are presented from a *strange-wave* shock-flame interaction case in air-ethylene.

1 Introduction

The development of accurate and efficient algorithms to simulate compressible reacting and general non-equilibrium flows based on the flux-vector and flux-difference splitting approach has been the subject of intense research since the early 80s. One of the most accurate and popular techniques available to date for the solution of hyperbolic problems is the Roe flux difference splitting. This technique requires the determination of an intermediate state - the Roe-average state- connecting the two sides of a Riemann. For arbitrary state equations, the Roe-average state is not unique. Colella and Glaz [3] proposed a solution algorithm for the Riemann problem in non-polytropic fluids with convex equation of state using as additional independent variable the equivalent of the polytropic exponent in an ideal fluid. Gleister [4] also proposed a linearised approximate Riemann solver for a convex equation of state in one dimension starting from Roe’s [16] original idea of using a parameter vector. Liu and Vinokur [11] extended various flux-splitting schemes (Beam and Warming [2], Steger and Warming [17] and van Leer [20]) and the approximate Riemann solver by Roe to non-equilibrium flows. Grossman and Walters [6] also proposed an extension of both van Leer’s

flux vector splitting and Roe's flux difference splitting schemes and implemented them in an implicit, cell-centred finite volume, three-dimensional Euler solver in curvilinear coordinates. Non-equilibrium chemistry was also accounted for by Leveque and Yee [10], who adopted a McCormack scheme with semi-implicit operator splitting to solve problems with stiff chemical sources. Grossman and Cinella [5] proposed a rigorous derivation of split-flux and split flux difference schemes based on Roe's approach for the computation of mixtures of ideal gases with vibrational equilibrium and finite-rate chemistry and demonstrated an implicit implementation of the scheme, albeit in one space dimension only. Jenny and Müller [7] proposed a Rankine-Hugoniot Riemann solver (RHR) to account for stiff source terms in the flux discretisation and presented computations of one- and two-dimensional laminar flames in an inviscid channel. Vinokur and Montagné [21] extend the flux vector (Steger and Warming [17] and van Leer [20]) and flux difference splitting (Roe) to the treatment of equilibrium real gases. Abgrall [1] extended the classic Roe's Riemann solver to mixtures in chemical equilibrium and showed also that the average state is not unique. Saurel et al [15] developed an exact Riemann solver for real gases and demonstrated its validity using the van der Waals state equation and a fifth-order virial state equation. Mottura et al. [13] reviewed a set of generalization of Roe's approximate Riemann solver to equilibrium real gases. They showed that on the basis of two-dimensional tests, all procedures (see literature cited above) yielded comparable results when coupled to a consistent procedure, based on local thermochemical equilibrium, to compute the fluid properties [12].

In this work an approach to the extension of the classic Roe's flux-difference splitting method is presented, which accounts for chemical non-equilibrium and allows a straightforward implementation in existing solvers. Firstly, it is shown that the excess internal energy arises naturally in the definition of the conversion Jacobians and in the eigenvectors of the semi-linearised Euler equations for a general, reacting gas mixture. The excess internal energy quantifies the deviation of the mixture from the behavior of a calorically perfect gas. The determination of the Roe's averaged state follows naturally from the definition of the Rankine-Hugoniot jump conditions across a discontinuity. The governing equations are linearised around a reference thermo-chemical state and the solution in terms of primitive variables is thus obtained as a first order correction by means of the appropriate conversion jacobians. It is shown that the Roe average state depends on a Roe-average composition and on the derivatives of the mixture compositions with respect to controlling variables. This feature makes the algorithm presented in this paper suitable to detailed scheme, as well as phenomenological schemes based on mixture fraction variables or progress rate variables.

2 Results

The chosen configuration (see [18]) is based on a shock tube with a total length of 6.94 m. The circular driver section with a diameter of 76 mm is filled with helium at a pressure of 15 bar. The test section has a cross section of $76 \times 38 \text{ mm}^2$. In the experiment, a 230 mm long window was fitted to grant optical access. The initial flame point was placed in the centre of the optical window, 135 mm from the end wall of the test section. The test section was filled with a 1:3:4 mixture of ethylene, oxygen and nitrogen at 100 Torr (about 0.134 bar). Ignition of the mixture is electrically driven. The spark was initiated before the diaphragm between the driver and testing section was pierced by an electrical cutter, in order to allow the formation of a sufficiently large flame kernel. The speed of the incident shock in the experiments was varied to obtain Mach numbers ranging from 1.5 to 2.5. In the present work an incident Mach number equal to 1.5 was selected for the simulations.

Initially, the interaction with the incident shock wave causes a slight deformation of the flame bubble, with

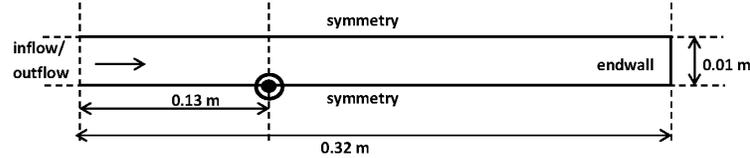


Figure 1: Computational domain.

the development of a Richtmyer-Meshkov instability. As time progresses, a *strange wave* as described by Khokhlov *et al.* [9] was observed. This type of interaction cannot be classified as a detonation wave, as its propagation speed is substantially lower than the theoretical Chapman-Jouguet value.

A detailed mechanism for fuels up to propane proposed in [14] has been employed here, consisting of 55 independent reactions to completion and 25 species. In contrast to previous studies on similar configurations (see for example [9]), no assumption has been made on the transport properties, which have been computed following [8].

The computational domain is similar to the one adopted by [9] and is represented in figure 1. A mesh featuring 1024×32 cells has been employed with a constant time step equal to $5e-8$ s. The simulation was carried out on 8 Intel Haswell CPUs (32 cores) and took 24 hours CPU time to complete. A further mesh, featuring 4 times as many cells in each coordinate direction has also been tested, requiring 4 weeks on the same number of cores to complete. The chemical reaction was initialised by imposing a temperature equal to 2400K in the region corresponding to the spark, located at 13 cm from the open boundary (fig. 1, left) with a radius of approximately 1.5 cm, centered on the lower symmetry boundary.

The first event shown in the experiment is the interaction between the burned mixture and the incident shock (travelling left to right). The interaction of the flame front with the incident shock takes place between 0.1486ms and 0.3292ms from the start of the experiment. The flame front is displaced and deformed by the shock. The temperature, density, and concentration fields are directly affected, as seen in Figure 2. Vorticity is generated at the left and right flame fronts because the shock crosses there a gradient inclined to the shock itself. The configuration of the left front is affected both by the incident shock and by weak reflections generated when the incident shock reaches the right side of the flame. The interaction with the incident shock turns the initially semicircular burned area into a convoluted pattern with two vortical areas and a highly stretched region in between. This process corresponds to the transformation of a spherical flame into a smoke ring by action of a shock. The shape of the flame surface is therefore determined by Richtmyer-Meshkov instabilities, as documented by Thomas *et al.* [19]. The two vortical areas, generated at the two sides of the initial flame front by the incident shock persist for the entire duration of the simulation as two concentrated vortices. The chemical reactions and the flow field are tightly coupled in the flame bubble deformed by the incident shock. Both the upstream and downstream vortex sheets undergo secondary instability and ramificate further. The initial asymmetry of the density field also causes reflections between the two walls.

After passage of the reflected shock, Meshkov instabilities develop on the left side of the flame front, which starts propagating to the left side of the domain. The highly deformed flame front becomes an area of sustained chemical reactivity. The increased reactivity sustains the formation of a strange wave [19] which appears in the solution between 1.1408 and 1.1878ms from the start of the computation. The mixture



Figure 2: Time-sequence of temperature contours for an incident shock at $Ma = 1.5$. Colour legend: 65 levels, $min = 400K$, $max = 3600K$.

behind the strange wave is stationary, as can be inferred by the positions of the large vortices.

The nature of the waves crossing the domain is elucidated by Figure 3, where the pressure histories at the locations of Khokhlov's [9] probes G4, G6 and G8 (12.8 cm, 19.2 cm and 25.6 cm respectively) are displayed. The results presented in this paper match qualitatively and quantitatively those produced by Khokhlov *et al.* [9].

3 Conclusions

In this paper a coupled, implicit algorithm for reacting compressible flow has been introduced. The scheme is based on a modification of Roe's flux vector difference splitting and enjoys favourable conservation and shock resolution properties. The scheme is constructed by requiring that the Roe averages for quantities such as molecular weights, specific heats, sound speeds etc. meet the Rankine-Hugoniot relations. The resulting splitting is similar to the canonical Roe splitting for quantities such as density, velocity and enthalpy. The definition of the Roe-average speed of sound is more convoluted but results in a value which is

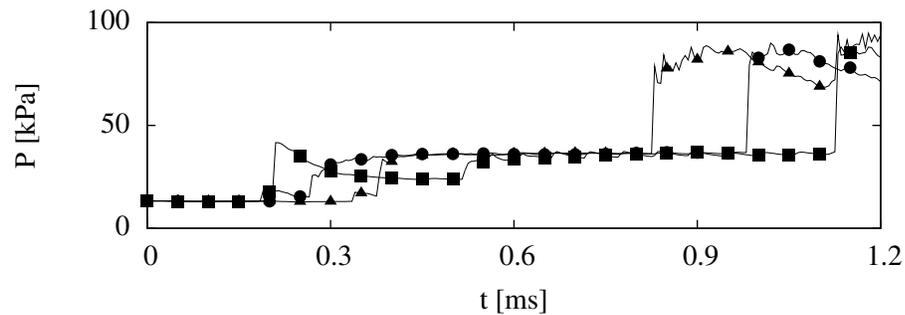


Figure 3: Time histories of static pressures at the walls. G4: ■, G6: ●, G8: ▲.

guaranteed to lie between the sound speeds of the left and right state. The scheme proposed allows a fairly straightforward construction of numerical fluxes and their jacobians if suitable representations are available for the thermodynamic mixtures of the gas mixture. The method has been applied to the simulation of the well-known flame-shock interaction experiment of Thomas *et al.* [18] and has been proved capable of capturing the salient features of the transition from deflagration to detonation. In particular the wrinkling of the initially spherical flame front and the appearance of Richtmyer-Meshkov instabilities has been accurately predicted.

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