Numerical Simulation of Compressible Reactive Viscous Flow in Complex Geometries

M. Manna[a], F. Marra[b1], A. Pascarelli[b2]
[a] *Dip. di Ingegneria Meccanica per l'Energetica, Universitá di Napoli "Federico II', Italy*
[b] *Istituto di Ricerche sulla Combustione - CNR, via Diocleziano 328, 80124 Napoli, Italy*

Abstract

The work presented here is mainly concerned with the ability of an inviscid flow model to capture the correct physical behaviors of the Detonation and Deflagrations to Detonations Transition (DDT) process. Inviscid and viscous numerical results concerning the detonation front propagating over a sudden expansion and in an obstacle filled channel are presented. The analysis provides a transparent and revealing qualitative and quantitative understanding that the usual arguments employed to support the validity of the inviscid flow model become increasingly weaker in a reactive environment.

Introduction

This work focus on a particular aspect of the numerical simulation of compressible reactive flows, and more specifically attempts to assess the validity and shortcomings of the inviscid flow model to study detonation and transition of fast deflagrations to detonations (DDT). From many experimental works it is known that an inflammable mixture may generate very fast flames which can lead to extremely dangerous detonations. This scenario is strongly influenced by the presence of complex geometries, and is thus of great relevance with respect to safety issues. Indeed, most of the available numerical studies are limited to the solution of the Euler equations, neglecting the viscosity related effects, with the usual argument that for high speed flows the Reynolds number is likely to be very high. However, the presence of complex and congested environment, as normally encountered in industrial plants, always implies local flow regions where viscous effects are important.

A comparison of detailed computations of a detonation front propagating over a sudden expansion both with the Euler and the Navier-Stokes models is presented to investigate the possible differences. Of course, the comparison is justified if the Euler model is assumed as a valid approximation of the real flow at high Reynolds number and the Navier-Stokes flow is computed at such a Reynolds number. Constraint are imposed on the allowable Reynolds number by the competitive effects of the grid size required for the resolution of small scale flow regions and the computational effort needed to solve the problem on very fine grids.

The comparison is then extended to a more complicated geometry constituted by a channel whit several wall mounted obstacles. This allow to identifies zones and complex flow structures where the viscosity mainly affects the behaviour of the detonation wave propagation.

Numerical Method

The flow fields are governed by the two-dimensional compressible reactive Navier-Stokes equations which read:

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_k}\left(\rho u_k\right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho u_i\right) + \frac{\partial}{\partial x_k}\left(\rho u_i u_k + p\delta_{ik}\right) = \frac{\partial}{\partial x_k}\left(\tau_{ik}\right) \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho e_t\right) + \frac{\partial}{\partial x_k}\left[\left(\rho e_t + p\right) u_k\right] = \frac{\partial}{\partial x_k}\left(\tau_{ik} u_i\right) - \frac{\partial}{\partial x_k}\left(q_k\right) \tag{3}$$

[1]Correspondig author, e-mail: marra@irc.na.cnr.it
[2]Present Address: INSEAN - Italian ship model basin, via di Vallerano, 139 - 00128 Roma, ITALY

$$\frac{\partial \rho Y}{\partial t} + \frac{\partial \rho u_k Y}{\partial x_k} + \frac{\partial j_k}{\partial x_k} = \omega \tag{4}$$

$$\tau_{ik} = \mu \left(2S_{ik} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ik} \right) \quad ; \quad S_{ik} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right)$$

$$q_k = -\frac{c_p \mu}{Pr} \frac{\partial T}{\partial x_k} \quad ; \quad j_k = -\rho D \frac{\partial Y}{\partial x_k} \quad ; \quad \omega = \rho \left(1 - Y\right) K \quad ; \quad K = A \exp\left(\frac{-E}{p/\rho} \right)$$

where standard tensor notation has been employed. In the previous relations the quantities ρ, u_i, e_t, p, T, Y are the density, the velocity components, the total energy per unit mass $\epsilon + u_k u_k/2$, the pressure, the absolute temperature, and the reaction progress variable respectively. The viscosity μ, the specific heats, the molecular diffusion coefficient D, the pre-exponential factor A and the activation energy E, are all assumed constant. The gas is assumed to be calorically perfect obeying the following equation of state:

$$\epsilon = c_v T = \frac{p}{\rho(\gamma - 1)} - QY \tag{5}$$

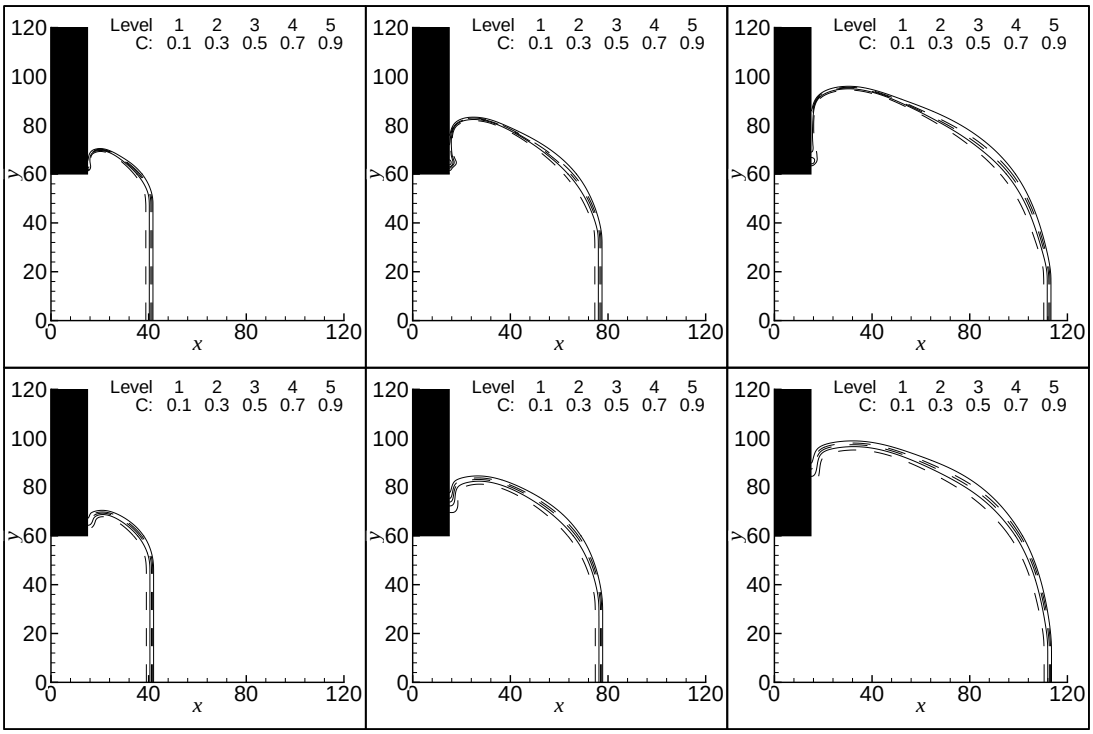

Figure 1: Progress variable iso-lines for Euler (top) and Navier-Stokes (bottom) calculation; frames from left to righ at times $t = 5, 10, 15$.

Constant Prandtl number and unitary Lewis number are assumed. Following the classical finite volume formulation the integral form of eq. (1–4) is discretized on a set of non overlapping quadrangular elements. The flow solver enjoys the flexibility of a patching domain decomposition technique with conformal interfaces. The convective terms are evaluated by means of an approximated Riemann solver whose interface values are obtained through a quadratic reconstruction procedure according to the MUSCL approach. The limiter function is applied to the characteristic variables. The diffusive terms are centrally discretized on a dual grid. Time advancement is carried out with a TVD Runge-Kutta scheme. The physical domain is discretized with H-type grids. Additional details concerning the flow solver can be found in [2].

Results

Numerical results are presented for the Chapman–Jouget detonation diffracting around a 90° corner, both for the reactive Euler and Navier-Stokes equations. Here a Reynolds number of 5000 based on the detonation velocity and expansion entrance length is adopted, so that, with a mesh of 3.6×10^5 points, the simulation may be considered resolved. The test problem describes the spatial-temporal evolution of a one-dimensional detonation front with particular emphasis on the dynamics of the acoustic and reaction waves. The initial states are obtained from a separate one dimensional computation of a fully reactive plane discontinuity front for the Euler equations whose relevant parameters are the wave velocity D_{CJ} and the heat release Q. They have been set to 7.1247 and 25, respectively. The medium ahead of the wave front is uniform and constant ($\rho = 1$, $u = v = 0$, $p = 1$). The solution of the 1-D problem after ten time units is plugged into the two dimensional domain so that the position of the detonation front is $x = 14$ (the corner is located at $x = 15$). The physical domain Ω is defined as $\Omega = \Omega_1 \cup \Omega_2$ with $\Omega_1 = [0, 120] \times [0, 60]$ and $\Omega_2 = [15, 120] \times [60, 120]$. The computational domain consists of two sub-domains corresponding to Ω_1 and Ω_2 with 600×300 and 525×300 uniformly spaced grid points, respectively. The computations are carried out till $t = 16$ with a Courant number of 0.8. The above described numerical test-case is the same as that adopted in [1], and the presented inviscid results compare very well. Figure (1) shows the isolines of the progress variable Y at

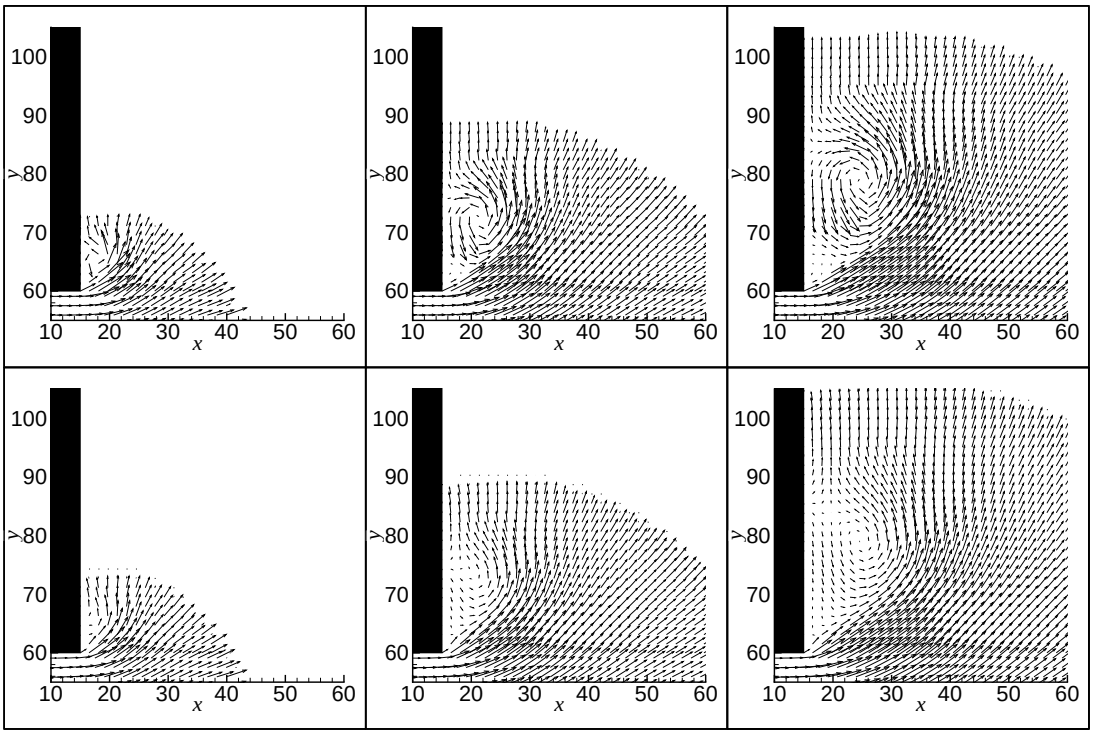

Figure 2: Velocity vectors in the near corner region; frames from left to right at times at $t = 5, 10, 15$; Euler (top), Navier-Stokes (bottom). The grid has been coarsened three times in both directions.

three different time levels ($t = 5, 10, 15$ s), as obtained integrating the reactive Euler and Navier-Stokes equations. The contour levels are separated by the same incremental value ($\Delta Y = 0.2$). Although the distributions show a similar path of development both in terms of extension and shape of the reaction front, a close inspection of the data reveals significant differences in the corner region. In particular there is a clear tendency of the inviscid calculation to under-predict

the reaction rate, a fact that, at first glance, seems counter-intuitive. Taking a closer look at the near corner flow fields distributions (see figure (2)) we found out that both solutions exhibit a fairly large separated region characterized by a primary vortical structure underneat a separating shear layer originated at the corner. The viscous solution shows a secondary counter-rotating vortex sitting below the primary. Note that the strength of the primary vortical structure is substantially larger in the inviscid case, although the gross size of the bubble is, roughly speaking, equal. In figure (3) we report the one dimensional distribution of the primitive variables ρ, v, T, Y extracted out of the two dimensional fields at a $y = const$ location crossing the primary vortex core (viz. $y = 77$ and $y = 75$ for the inviscid and viscous solution respectively).

The figure clearly shows that in the near wall region there is a thin layer where the progress variable barely exceeds 0.5 in the Euler calculation, while the viscous solution indicates that the reaction is completed therein. The wall values of the progress variable are $Y_w = 0.51$ and $Y_w = 0.98$ for the Euler and Navier-Stokes solutions respectively. There are two main mechanisms responsible for such behavior, viz. the strength of the Prandtl-Meyer expansion (determining the pressure level within the separated region), and the intensity of the reverse (with respect to the main motion direction) flow behind the step. While both phenomena can hardly be conceived outside of the Navier-Stokes context, they are indeed reproduced (at most) qualitatively by the inviscid calculations, thanks to the inherently dissipative character of the numerical scheme, a necessity when dealing with weak solutions of systems of conservation laws. In the present example the advance of the flame front is delayed (!) by the stronger intensity of the vortex circulation in the inviscid case, which is witnessed by the larger negative velocity peak at $x = 20.6$. The net result of the near corner viscous separation is a considerable decrease of the distance between the leading shock wave and the reaction front. At $t = 15$ in the upper left zone of the physical domain the above mentioned distance decreases from 6 for the Euler case to 4 in the viscous one (results not shown).

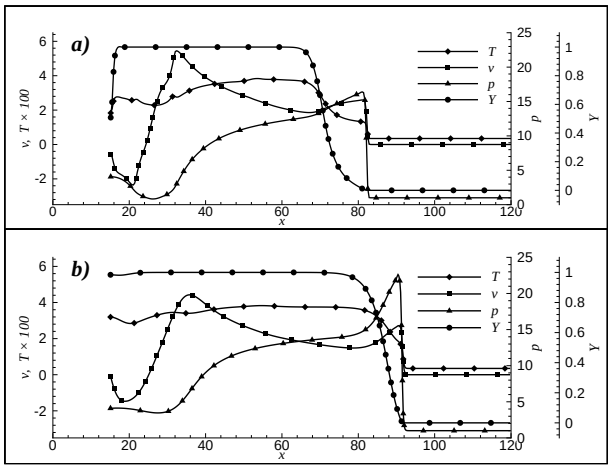

Figure 3: Progress variable Y, pressure p, velocity v and temperature T distribution at $t = 15$; Euler (top $y = 77$), Navier-Stokes (bottom $y = 75$)

Preliminary results are here presented for the propagation of a detonation wave in a channel with several wall mounted obstacles. The geometry and initial conditions resamble that adopted in a previous investigation of shock wave propagation in an inert gas [3]. The following expression for the source term of the progress variable equation (4) has been adopted:

$$\omega = \rho^3 (1 - Y)^3 K_1 K_2$$

where

$$K_1 = A \exp\left(\frac{-E}{p/\rho}\right), \quad K_2 = \frac{1}{\tau_{chem}} \mathcal{H}(p/\rho R - T_{ign})$$

$\mathcal{H}$ being the Heaviside function. The results show that a general qualitative agreement is observed for the two simulations. However quantitative analysis reveals that differences up to 34 % in the maximum Mach number, 5 % in the maximum temperature and 8 % in the maximum pressure, are obtained in the regions of highest shear and detonation/wall interaction.

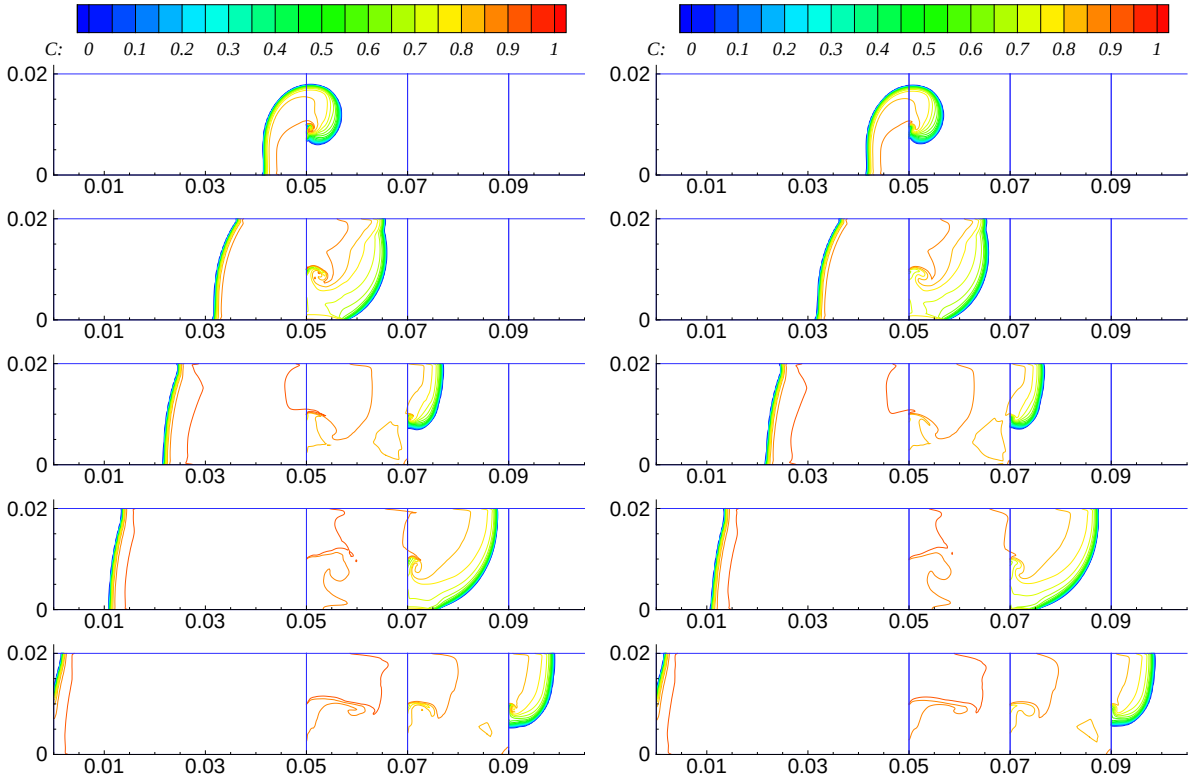

Figure 4: Progress variable contours in the channel with obstacles; Euler (left), Navier-Stokes (right).

Conclusions

Detailed computations of a detonation front propagating over a sudden expansion and in a channel with obstacles have been carried out both with the Euler and the Navier-Stokes models, revealing substantial differences. The data clearly indicate that the usual arguments employed to support the validity of the inviscid flow model become increasingly weaker in a reactive environment, a fact that may have deep implications in the context of the prediction of accidental explosions.

Although the Euler equations provide a satisfactory level of predictivity in unbounded domains, the interaction with bluff bodies induce local phenomena, like unsteady separation, that may strongly affect the evolution of reactive fronts.

References

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