HIGH ORDER NUMERICAL SCHEMES WITH POSITIVITY-PRESERVING PROPERTIES FOR THE SOLUTION OF THE TRANSPORT EQUATIONS IN REACTIVE FLOWS

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1. Introduction.

One of the most important themes of research in Computational Fluid Dynamics concerns the simulation of flows in which the transport variables have so strong gradients to result practically irresolvable on a given mesh. In these cases, indeed, the simulation requires a careful treatment of the advective terms. This is due to the fact that, often, in practical problems these flows have a strong non-linear component that is mainly driven by the advection. Facing out transport problems with strong variable gradients, it is useful to remark that one of the most important and delicate area of research deals with the numerical simulation of inviscid flows whereas the solution can loose its regular character due to the formation of shocks so that it must be considered in a weak form. Consequently, inviscid problems are a deep source of fundamental probes even for viscous problems. However, as in this paper we focus only on viscous flows at low Mach number, we will not go inside important themes (as the preservation of the entropy condition or the assignment of compatible sets of boundary conditions, whose an exhaustive description is given in: [1], [2]). In fact, we will mainly focus on the problem of avoiding numerical oscillations of the solution because, for reactive flows, these oscillations can lead to unphysical values of some transport variable (e.g. mass fraction) that can fall out of its range of values.

2. The theoretical framework.

In an important paper of Godunov [3], it was shown that linear schemes having the property of not generating new extrema (monotone scheme) can be at most first-order accurate (Godunov's theorem). This has been, for a long time, one of the main reasons for which first-order upwind schemes have been a work-horse in many applications. On the other hand, numerical solutions of flows at high Reynolds number, due to the poor accuracy, can not be obtained resorting to first-order schemes, as it can be shown simply by solving the linear one dimensional wave equation (e.g. see [4]). Indeed, for reacting flow simulations, the artificial numerical viscosity added to the fluid molecular viscosity acts to over-smooth sharp gradients and this is source of heavy errors because the presence of such numerical viscosity results in unphysical higher reaction conversion rates (as good review of numerical approaches for reacting flows see: [5]). Thus one must resort to higher order schemes that, if linear, generate numerical oscillations.

In general, to get around the Godunov's theorem, one must use non linear high order schemes even for linear problems. Two general strategies are possible: the first consists in "preventing" the generation of numerical oscillations by acting on the production mechanism, while the second consists in "damping" the generated oscillations by using *ad hoc* artificial dissipation terms. In this paper we will adopt the first approach due to the fact that it is best suitable to be applied with the class of high order upwind schemes we will use in the framework of a Control Volume formulation. In the following, we will essentially exploit some correction factors called "limiters" applied to the computed numerical advective fluxes.

3. Monotonicity condition and positivity preserving properties.

Let us first briefly recall some important definitions. Consider the scalar one dimensional transport equation:

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0 \qquad (1)$$

where *u* is the constant positive advection velocity. The exact solution of this problem is given by:

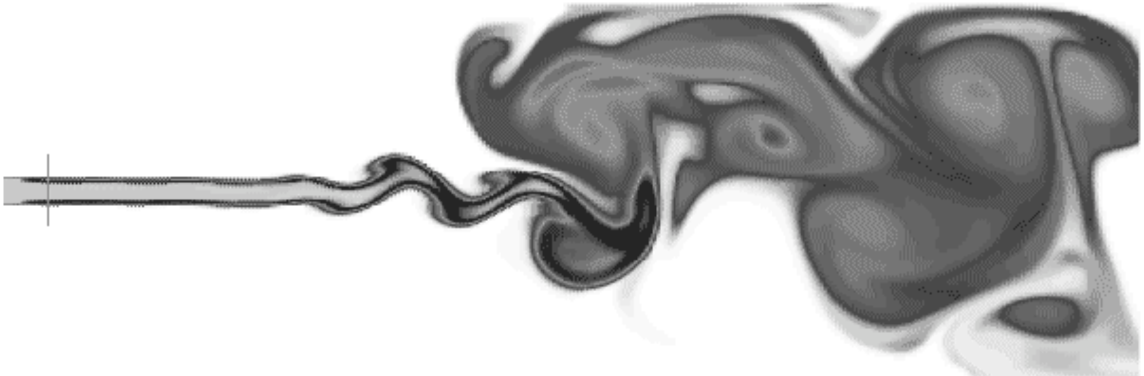

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Fig. 2. Shaded contours and cross section plot of mass fraction. Solutions obtained with present high order scheme: a) Unlimited scheme, b) Scheme with FCT-like procedure.

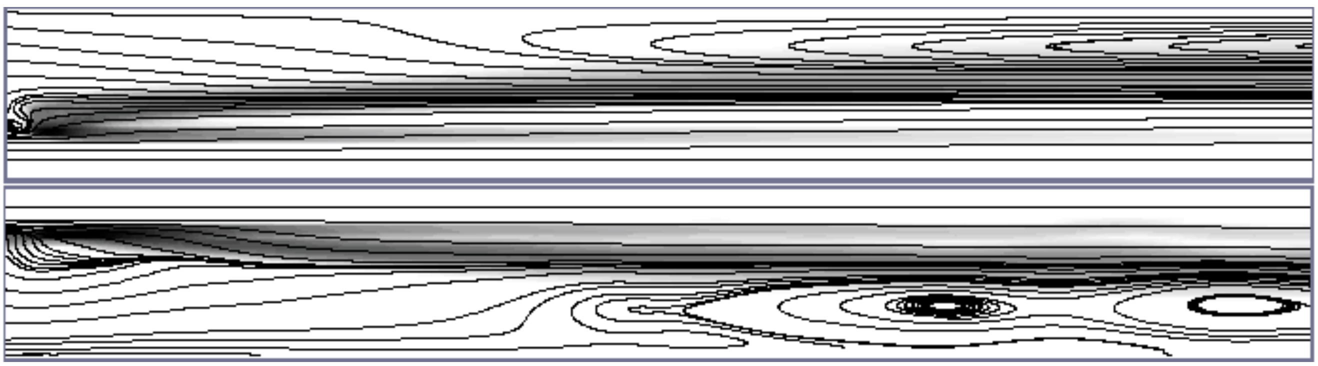

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Fig. 3. Simulation of reacting flow on axis-symmetrical domain. The reaction rate and stream-lines pattern are shown in a mirror image with respect to first order scheme (upper) and present high order scheme (lower).

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