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SHORT COMMUNICATION

SIMULATION OF PLANAR HIGH SPEED COMBUSTION PHENOMENA

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ABSTRACT

A modified version of an essentially non-oscillatory high resolution scheme is applied to the simulation of two-dimensional combustion waves. Through the splitting of the governing equations the method is applied to the homogeneous system and the source terms are approximated by means of a Runge-Kutta third-order scheme. The results obtained in the modelling of a high speed wave show an improvement with respect to a semi-implicit scheme in the reconstruction of the shock propagation.

KEY WORDS Non-linear conservation laws Detonation waves Conservative schemes High resolution methods

INTRODUCTION

The combustion waves, sustained by the coupling between chemical kinetics and gas-dynamics, are governed by the classical gas-dynamic (compressible Navier-Stokes) equations completed with source terms modelling the chemistry. Nevertheless, in the investigation of high speed phenomena, diffusive terms are usually neglected[1]. Numerical difficulties concerning the reconstruction of shocks and the simultaneous occurrence of small (chemical) and large (hydrodynamical) time scales often arise in the discrete modelling of such phenomena. The resolution of the computational grid assures a better reconstruction of the shocks and avoids numerical instability. Often, however, severe limitations are imposed by computational costs which do not permit the use of arbitrarily small time and space steps.

Semi-implicit methods which use a space-staggered mesh and whose stability does not depend on the sound speed have been proposed for the numerical solution of hyperbolic systems[2-4]. In this way, accurate results are obtained at a reduced computational cost. Anyway, an unsatisfactory reconstruction of the shock propagation velocity may be observed, mostly due to the not fully conservative formulation of the numerical scheme. This difficulty may be overcome by means of ENO (essentially non-oscillatory) high resolution schemes, which in the recent years have been intensively applied to the approximation of conservation laws[5-7]. A splitting of the governing equations allows separate integration of the reactive terms.

In this paper an ENO scheme proposed by Osher in Reference 7 is applied to the simulation of planar high speed combustion waves. The governing equations of planar combustion phenomena

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are given in the next section. The numerical method is described in the following section and the numerical results obtained on some test problems are presented in the fourth section.

GOVERNING EQUATIONS

In the following a mathematical model for a two-component mixture (burnt and unburnt gases) will be considered. It is supposed that the unburnt gas is converted into burnt gas by a one-step irreversible chemical reaction; the absolute temperature T is assumed to be the same for both species, which behave like an ideal gas. If external forces and diffusive terms are neglected, the governing equations may be expressed in vectorial form as:

$$\mathbf{w}_t + \mathbf{f}(\mathbf{w})_x + \mathbf{g}(\mathbf{w})_y = \mathbf{S}(\mathbf{w})$$

where:

$$\mathbf{w} = (\rho, \rho u, \rho v, \rho E, \rho Z)^T$$
$$\mathbf{f}(\mathbf{w}) = (\rho \mathrm{u}, \rho u^2 + p, \rho uv, u(\rho \mathrm{E} + p), \mathrm{u}\rho Z)^T$$
$$\mathbf{g}(\mathbf{w}) = (\rho v, \rho uv, \rho v^2 + p, v(\rho E + p), v\rho Z)^{\mathrm{T}}$$
$$\mathbf{S}(\mathbf{w}) = (0,0,0,0,\rho Z S)^T$$
$$E = p/(\rho(\gamma - 1)) + (u^2 + v^2)/2 + qZ,$$

and the ideal gas equation of state

$$pm = \rho RT$$

is valid. The variables ρ, u, v, E, p, are the density, the Cartesian velocities, the specifical internal energy and the pressure of the mixture, respectively; R is the universal gas constant; Z is the mass fraction of the reactant; q is the heat released by the chemical reaction; γ and m are the specific heats ratio and the molar mass, respectively, supposed to be equal for burnt and unburnt gas. The Arrhenius type source term $\mathbf{S}$ is assumed, as customary, to be an exponential function of the temperature[1]. Suitable initial and boundary conditions must be specified.

The Jacobian matrices $\mathbf{A} = \mathbf{f}(\mathbf{w})_{\mathbf{w}}$ and $\mathbf{B} = \mathbf{g}(\mathbf{w})_{\mathbf{w}}$ of (1) are given by

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ (\gamma-1)v^2/2 + (\gamma-3)u^2/2 & (3-\gamma)u & (1-\gamma)v & \gamma-1 & (1-\gamma)q \\ -uv & v & u & 0 & 0 \\ uK & (1-\gamma)(u^2-v^2)/2 - K & (1-\gamma)uv & \gamma u & (1-\gamma)uq \\ -uZ & Z & 0 & 0 & u \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ -uv & v & u & 0 & 0 \\ (\gamma-1)u^2/2 + (\gamma-3)v^2/2 & (1-\gamma)u & (3-\gamma)v & \gamma-1 & (1-\gamma)q \\ vK & (1-\gamma)uv & (1-\gamma)(v^2-u^2)/2 - K & \gamma v & (1-\gamma)vq \\ -vZ & 0 & Z & 0 & v \end{bmatrix}$$

where

$$K=(\gamma-1)(u^2+v^2+qZ)-\gamma E$$

The matrices of the eigenvalues and right eigenvectors of **A** are

$$\Lambda_A=\mathrm{diag}(u-c,\ u,\ u,\ u,\ u+c)$$

and

$$\mathbf{R_A}=\begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ u-c & u & 0 & 0 & u+c \\ v & v & 1 & 0 & v \\ H-uc & (u^2+v^2)/2 & v & q & H+uc \\ Z & 0 & 0 & 1 & Z \end{bmatrix}$$

respectively, where $c=(\gamma p/\rho)^{1/2}$ is the sound speed and

$$\mathrm{H}=(u^2+v^2)/2+qZ+c^2/(\gamma-1).$$

The structure of the corresponding matrices for **B** is similar:

$$\Lambda_B=\mathrm{diag}(v-c,\ v,\ v,\ v,\ v+c)$$

$$\mathbf{R_B}=\begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ u & 1 & u & 0 & u \\ v-c & 0 & v & 0 & v+c \\ H-vc & u & (u^2+v^2)/2 & q & H+vc \\ Z & 0 & 0 & 1 & Z \end{bmatrix}.$$

The columns of $\mathbf{R_A}$ ($\mathbf{R_B}$) constitute a set of linearly independent vectors so that the system (1) may be decomposed into local characteristic fields.

NUMERICAL INTEGRATION

In the numerical integration of conservation laws the recently developed ENO schemes have proved to be very accurate in the approximation of flux derivatives. They use a local adaptive set of points, chosen according to the order of the method and the characteristic directions to obtain information from regions where the solution is smooth. In this way, high order accuracy guarantees a sharp non-oscillatory shock reconstruction[6,7]. As regards the reaction term appearing in (1), it may be necessary to increase the resolution, as suggested in References 8 and 9, owing to the strong non-linearity in the temperature and the fact that the chemical time scale may be orders of magnitude faster than that of the fluid dynamical. In the present paper a splitting technique for the integration of Equation (1) is proposed. The associated homogeneous system is integrated by means of a simplified but still conservative version of the ENO schemes, that is ENO-LLF presented in Reference 7, which seems to be easy to implement and yet guarantees the entropy condition satisfied[10]. The stiff term modelling the chemistry is solved by a Runge-Kutta third-order scheme.

The implementation of an ENO scheme on a system of conservation laws requires its decomposition into local characteristic fields with the help of left and right normalized eigenvectors of its Jacobian matrices **A** and **B**[11].

On a computational grid $x_i = i\Delta x$, $y_j = j\Delta y$, at each $t_n = n\Delta t$, let $\mathbf{A}_{i+1/2,j}$ denote the Roe averaged Jacobian[12] in $x_{i+1/2}$, y_j and $(\lambda_{i+1/2,j})^k$, $(\mathbf{l}_{i+i/2,j})^k$, $(\mathbf{r}_{i+1/2,j})^k$, $k = 1, \ldots, 5$, its eigenvalues and left and right normalized eigenvectors, respectively. The ENO interpolation of the "characteristic fluxes" $(\mathbf{l}_{i+i/2,j})^k \cdot \mathbf{f}(\mathbf{w}(x_{i+1/2}, y_j))$, requires the computation of divided difference tables of $\mathbf{f}(\mathbf{w})$ and $\mathbf{w}$ to a fixed order r and the construction, on a set of points chosen according to the smallness of differences and the characteristic directions given by $(\lambda_{i+1/2,j})^k$, of interpolating polynomials of order r of the "characteristic fluxes". In this way a numerical approximation $(f_{i+1/2,j})^k$ of the transformed fluxes is obtained. The numerical original fluxes $\mathbf{f}(\mathbf{w}(x_{i+1/2}, y_j))$ are then reconstructed by means of the right eigenvectors

$$\mathbf{f}(\mathbf{w}(x_{i+1/2}, y_j)) = \sum_{k=1,5} (\mathbf{f}_{i+1/2,j})^k (\mathbf{r}_{i+1/2,j})^k.$$

The space derivative $\mathbf{f}(\mathbf{w})_x$ is then approximated at each computational point by centred differences

$$\mathbf{f}(\mathbf{w}(x_i, y_j))_x \equiv (\mathbf{f}(\mathbf{w}(x_{i+1/2}, y_j)) - \mathbf{f}(\mathbf{w}(x_{i-1/2}, y_j)))/\Delta x.$$

An analogous procedure has to be applied to the computation of $\mathbf{g}(\mathbf{w}(x_i, y_j))_y$. The integration of the differential terms is completed by time discretization, according to a multilevel Runge-Kutta method. The same Runge-Kutta scheme is adopted for the approximation of the splitted reactive source term.

It may be observed that the splitting technique can be applied also to the treatment of diffusive terms, if taken into account.

TEST PROBLEMS

The accuracy and the efficiency of the proposed numerical method (ENO-SPlitted) has been tested on two test problems: a one-dimensional Chapman-Jouguet wave travelling in a plane region[13] and, as a more significant two-dimensional problem, a diluted stoichiometric oxyhydrogen mixture in a narrow channel.

For the first example, the initial conditions correspond to the steady exact solution of a one-dimensional Chapman-Jouguet wave. Such detonation is assumed to have a relatively small heat release ($q = 6.9283 \times 10^9$ erg/g) and is modelled on initial data for the preshock state corresponding to 25 per cent ozone and 75 per cent oxygen at about room temperature. Null normal derivatives on the horizontal boundary are assumed. Pressure, density, velocity components of the mixture and mass fraction of the reactant are taken to be

$$(p_0, \rho_0, 0, 0, 1), \qquad x > 0$$
$$(p_1, \rho_1, u_1, 0, 0), \qquad x \leq 0, \ \forall y,$$

where $p_0 = 8.32083 \times 10^5$ dyne/cm^2, $\rho_0 = 1.201 \times 10^{-3}$ g/cm^3, while p_1 and ρ_1 are evaluated from the Rankine-Hugoniot conditions. The horizontal velocity of the burnt gas is $u_1 = (\rho_1 - \rho_0) \cdot (\gamma p_1/\rho_1)^{1/2}/\rho_0$, where for the specific heat ratio the value $\gamma = 1.4$ is assumed. Finally, in modelling the chemistry

$$S = -k_0 H(T - T_c)$$

is assumed, where $k_0 = 6.22885 \times 10^9\ s^{-1}$, $T_c = 500$K and H is the Heavyside step function[8].

A semi-implicit non-conservative scheme (SINC) described in Reference 14 has been also applied to the same problem for a comparison. The results obtained by ENO-SP are in agreement with the ones reported in References 8 and 15 relative to a one-dimensional Chapman-Jouguet wave: the computed pressure reveals the expected sharp reaction zone, with a peak of about

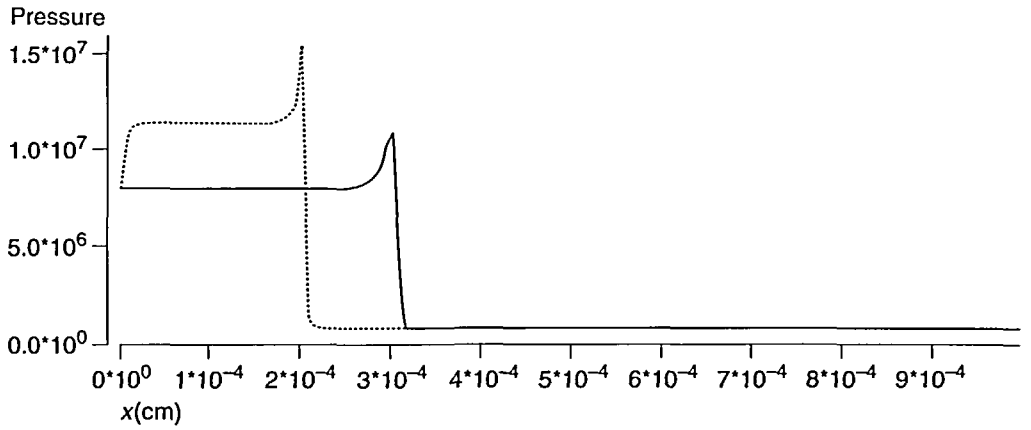

Figure 1 Pressure at $t = 0.5 \times 10^{-8}$ s

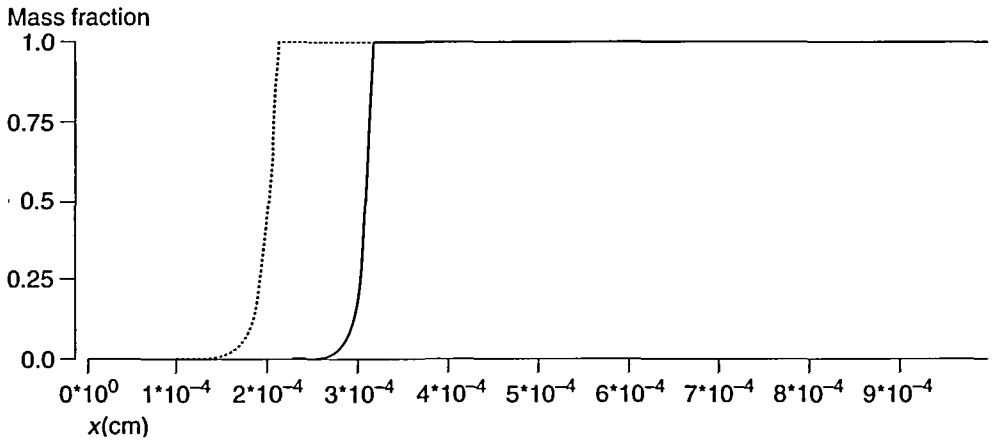

Figure 2 Mass fraction at $t = 0.5 \times 10^{-8}$ s

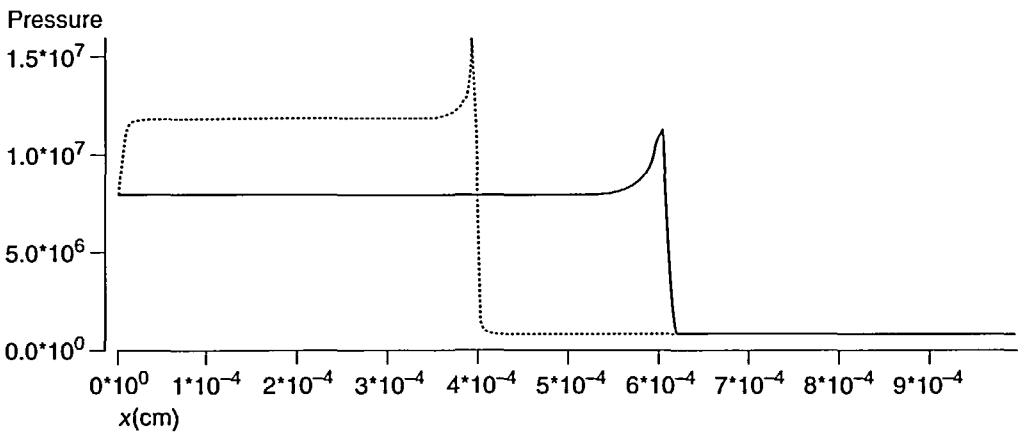

Figure 3 Pressure at $t = 10^{-8}$ s

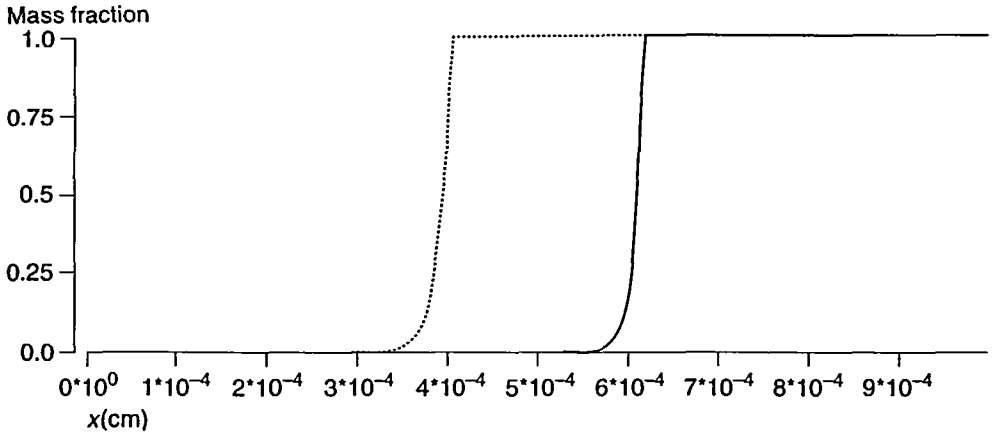

Figure 4 Mass fraction at $t = 10^{-8}$ s

12atm. Moreover, the shock propagates at the expected velocity $U = \rho_1 u_1 (\rho_1 - \rho_0)$ (Chapman-Jouguet detonation velocity). The better performance of ENO-SP with respect to SINC in the reconstruction of the shock propagation velocity and the peak value for the pressure is mostly due to the conservative formulation, whose importance for high velocity combustion problems is underlined in Reference 16.

The computed pressure and mass fraction, which as expected do not depend on the y co-ordinate, are reported in Figures 1-4 for two different times. They have been obtained on a grid of 200×10 points with a time step $\Delta t = 5 \times 10^{-12}$. The continuous and dashed lines correspond to ENO-SP and SINC methods, respectively.

In the second problem, a diluted stoichiometric oxyhydrogen mixture (6.25 per cent hydrogen, 50 per cent oxygen and 43.75 per cent helium) in a narrow rectangular cross section is considered[17,18]. In this case the reaction term reads

$$S = -KZp^2\{\exp(-E_a/RT) - \exp(-(E_a+q)/RT)\}$$

where

$$K = 10^{-7} cm^3/g/\text{sec};$$

$$E_a = 13.9 \times 10^9 erg/g;$$

$$q = 4 \times 10^{10} erg/g.$$

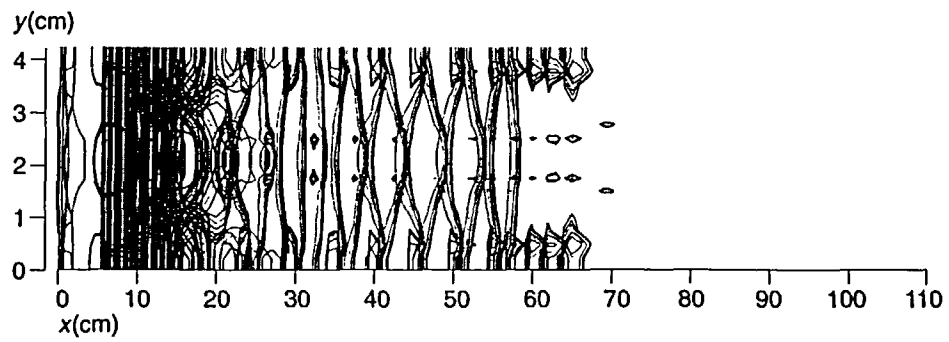

Figure 5 Evolution of pressure contour lines at $t = 0.42 \times 10^{-3}$ s

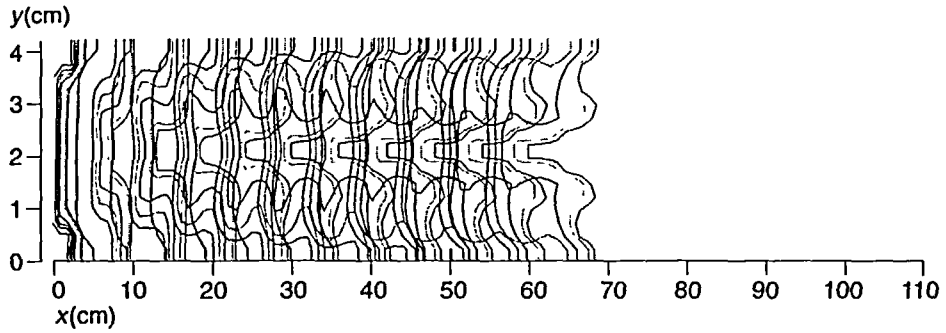

Figure 6 Evolution of mass fraction contour lines at $t = 0.42 \times 10^{-3}$ s

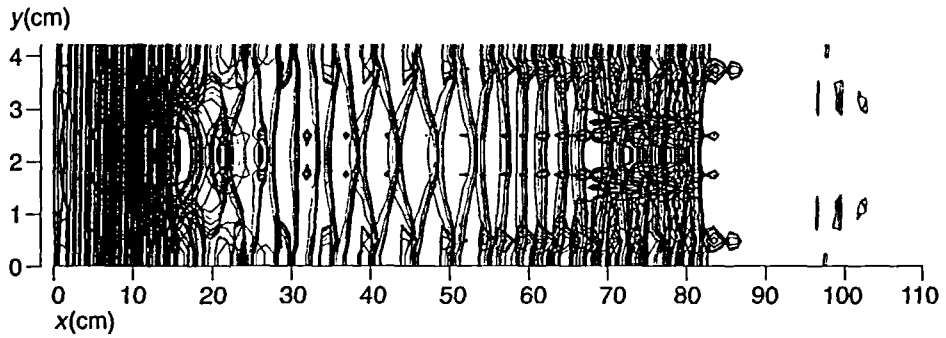

Figure 7 Evolution of pressure contour lines at $t = 0.6 \times 10^{-3}$ s

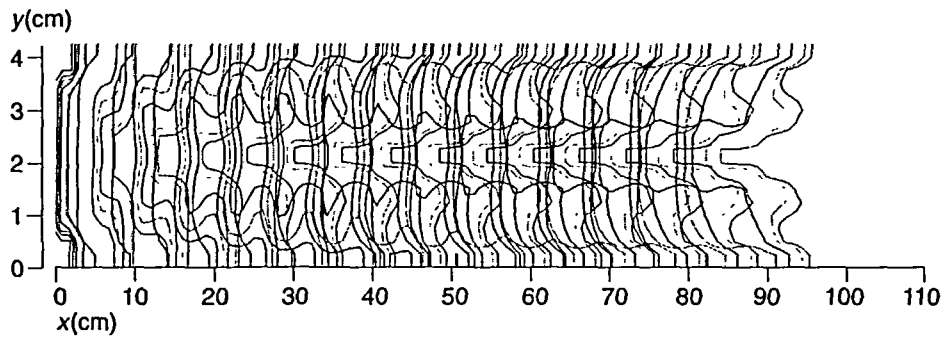

Figure 8 Evolution of mass fraction contour lines at $t = 0.6 \times 10^{-3}$ s

Figure 8 Evolution of mass fraction contour lines at $t = 0.6 \times 10^{-3}$ s

A plane steady detonation propagating in the mixture is perturbed at $t = 0$ by a pocket of unburnt gas placed perpendicular to the direction of wave propagation, causing the growth of instabilities which lead to transverse shock waves. The result is an equilibrium configuration repeating at equally spaced intervals as the detonation propagates in the channel.

A computational space grid of 150 × 20 points and a time step chosen according to the CFL condition are assumed. Contour lines for the pressure and mass fraction of the reactant computed by means of ENO-SP show the expected configuration, as may be seen in Figures 5-8.

CONCLUSIONS

In this paper an accurate numerical model for two-dimensional combustion waves has been presented. A splitting of the governing equations allows the approximation of the differential terms by means of an ENO scheme and the source terms by means of a Runge-Kutta third-order scheme, so that the method proposed gives the same accuracy as in Reference 15 at a lower computational cost, since the splitting of the system avoids the computation of the derivatives of the source terms with respect to all the unknowns. This may be an advantage in particular in problems where several complex chemical reactions are taken into account. Of course in some cases *ad hoc* integration techniques for source terms may be convenient. In our experience the proposed Runge-Kutta scheme has given satisfactory results on the examples described above[19].

The extension of the proposed method, both to three spatial dimensions and more complex fluid dynamical models, is in progress.

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