A COMPARISON OF TIME-SPLITTING AND PARTICLE METHODS FOR HIGH-SPEED FLOWS WITH CHEMICAL NON-EQUILIBRIUM

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Abstract. *The present work is concerned with the study of hypersonic reacting flow numerical methods. Two algorithms to couple the chemical non-equilibrium to the fluid dynamics are studied. In the first one, the coupling is achieved by Strang's time-step splitting procedure. In the second one, the chemical reaction process is defined for "finite quantities" moving through the stationary mesh. The detailed description of the use of "finite quantities" to represent the chemical processes is included in a companion paper also submitted to ENCIT-2008. The present paper concentrates in the comparison of advantages and disadvantages of the two different approaches for dealing with chemical non-equilibrium processes. The fluid dynamics is modeled by the Euler equations and the chemical reaction speeds by the Arrhenius law. Mixtures of ideal gases are considered. The thermodynamical data are based on JANNAF tables and Burcat's database. The algorithm proposed by Liou, known as AUSM+, is implemented in a cell-centered based finite volume method and in an unstructured mesh context. A multidimensional limited MUSCL interpolation method is used to perform property reconstructions and to achieve second-order accuracy in space. The minmod limiter is used. The time step is performed such that the fluid dynamics part is updated separately from the chemical part. The second order accuracy, five stage, Runge-Kutta time-stepping scheme is employed to perform the time march for the fluid dynamics. The numerical code VODE, which is part of the CHEMKIN-II package, is adopted to perform the time integration for the chemical reaction terms. Solutions generated with each algorithm are presented and compared. The freestream reacting fluid is composed of H_2 and air at the stoichiometric ratio. The configurations considered are the hypersonic flow over a wedge, in which the oblique detonation wave is induced by an oblique shock wave, and the hypersonic flow over a blunt body. Differences between the solutions obtained with each formulation are presented and discussed, including the effects of grid refinement in each case.*

Keywords*: Supersonic Combustion, Numerical Simulation, Wedge, Blunt Body.*

1. INTRODUCTION

The present paper and a companion paper, also submitted to ENCIT-2008, describe and validate a new hybrid Eulerian/Lagrangian formulation to simulate reactive hypersonic flows. The current paper concentrates in the comparisons of the hybrid methodology and the conventional Eulerian methodology. Solutions obtained with the two formulations are presented, compared and investigated. For the Eulerian methodology, the continuity, the momentum, the energy and the species equations are defined for stationary meshes. The coupling is achieved by Strang's time-step splitting procedure (Strang, 1968). For the hybrid methodology, the continuity, the momentum and the energy equations are defined for stationary meshes, whereas the chemical kinetics is defined for particles that move with the fluid.

First, Lehr's experiment for Mach number equal to 6.46 (Lehr, 1972) is simulated with the Eulerian methodology. Three meshes, different in format and refinement, are employed. Although the formulation is for unstructured grids, only structured quadrilateral meshes are used. The solutions are presented and compared to the experimental data. An investigation specifically concerned with the reactive mixture is carried out to clarify the challenges of simulating, with the Eulerian methodology, the oblique reaction front that progressively aligns to the local flow. For the hybrid methodology, the solutions are shown in the companion paper. Second, a reactive hypersonic flow around a wedge is simulated for both formulations. Two meshes, different in format and refinement, are employed. The solutions are presented, compared and analyzed. A second investigation, specifically targeting the reactive mixture, is carried out in order to clarify the characteristics of the solutions obtained with the Eulerian methodology corresponding to the position of the reaction front.

2. NUMERICAL FORMULATION

2.1. General Formulation

This item presents the formulation that is common for both approaches. The fluid dynamics is modeled by the Euler equations and the chemical reaction speeds by the Arrhenius law. Liou's upwind, flux vector splitting method (Liou, 1994, Liou, 1996), known as AUSM+, is implemented in a cell-centered based finite volume code for unstructured meshes. The reinterpretation of the formulation for unstructured meshes follows Azevedo and Korzenowski (1998). The

2nd-order spatial accuracy is obtained using the MUSCL reconstruction (van Leer, 1979) and the MINMOD limiter (Hirsch, 1988) to extrapolate the primitive variables from the centroid to the faces of the cells. The second-order accuracy, five-stage Runge-Kutta (Mavriplis, 1988, Mavriplis, 1990) scheme is employed to perform the time march. The VODE numerical code (Byrne and Dean, 1993) is adopted to perform the time integration for the chemical reactions. The reaction rate for each species is determined with the use of the CHEMKIN-II code (Kee *et al*., 1991). The thermodynamic properties are defined using polynomial tables of JANNAF (Anon, 1970) and Burcat's database (Burcat, 1984). The Balakrishnan and Williams (1993) chemical kinetics mechanism is selected to model the H_2 and air reactive mixture.

2.2. Eulerian Formulation

Euler equations include the continuity, the momentum, the energy and the species equations. Strang's time-step splitting procedure (Strang, 1968) is used for time advancement. The interested reader is referred to the work by Pimentel *et al.* (2002) for further details on the formulation.

2.3. Hybrid Eulerian/Lagrangian formulation

Euler equations include the continuity, the momentum and the energy equations. Species equations are not considered. Particles moving with the fluid carry the chemical composition information. The Eulerian/Lagrangian interface is conducted in a such way that the density, speed and the internal energy values of the particles are defined as being equal to the values of the control volume that contains the particle, whereas the mass fraction of the control volume is defined as being equal to the weight-averaged mass fractions of the chemical composition of the particles contained in the volume. The time advancement is achieved by three independently steps, one step for the fluid dynamics, one step for the chemical reaction process and one step for the particle position.

3. RESULTS AND DISCUSSION

3.1. Blunt Body

Lehr's experiment for Mach 6.46 (Lehr, 1972) is simulated with the Eulerian formulation. The flow is composed of a stoichiometric H_2-air mixture. The geometry is a sphere-cylinder of 15 mm diameter. The free stream conditions are T_∞ = 292 K and p_∞ = 320 mmHg. Simulations are carried out over three structured quadrilateral meshes. The boundaries of the meshes are presented in the Fig. 1. Grid 1 is composed of 20000 nodes and 19671 cells, in which the distribution is 80 × 250 points in the normal and longitudinal directions, respectively. The nodes are equally spaced in each direction. Grid 2 is composed of 30000 nodes and 29631 cells, in which the distribution is 120 × 250 points. The nodes are also equally spaced in each direction. Grid 3 is composed of 60000 nodes and 59451 cells, in which the distribution is 150 × 400 points. Specifically for the Grid 3, the nodes are not equally spaced in each direction. The density of nodes is greater in the region of the shock wave and the reaction front. In the direction normal to the body, from the entrance boundary to the wall, the distance between the nodes is linearly reduced from the first to the 75th node to 1/5 of the initial distance. From the 75th to 150th node, the distance is kept constant. In the longitudinal direction, from the exit to the symmetry boundary, the spacing between the nodes is linearly reduced from the first to the last node to 1/3 of the initial distance. Grid 1 and 2 are similar in refinement, but differ considerably in format. Grid 3 is much finer and comprises only the flow field around the semi-sphere leading edge. Position coordinates are in centimeters.

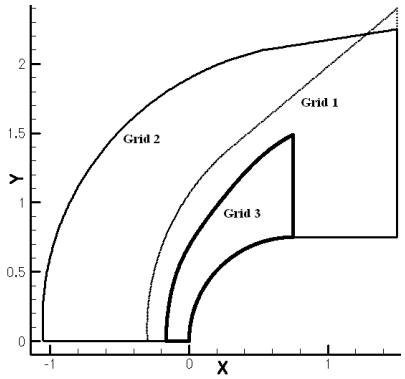

Figure 1. Borders of the meshes used to simulate Lehr's experiment for Mach 6.46 (Lehr, 1972); Grid 1 (80 × 250), Grid 2 (120 × 250) and Grid 3 (150 × 400).

Figure 2 shows the density and the H_2O mass fraction contours of the solutions obtained for the three meshes. For the solutions obtained with Grid 1 and Grid 2, the pattern observed in Lehr's experiment (Lehr, 1972) is not seen. It is not clear that the reaction front separates from the shock wave as the two fronts become more oblique. On the other hand, for Grid 3, it is possible to notice the beginning of the detachment of the two fronts.

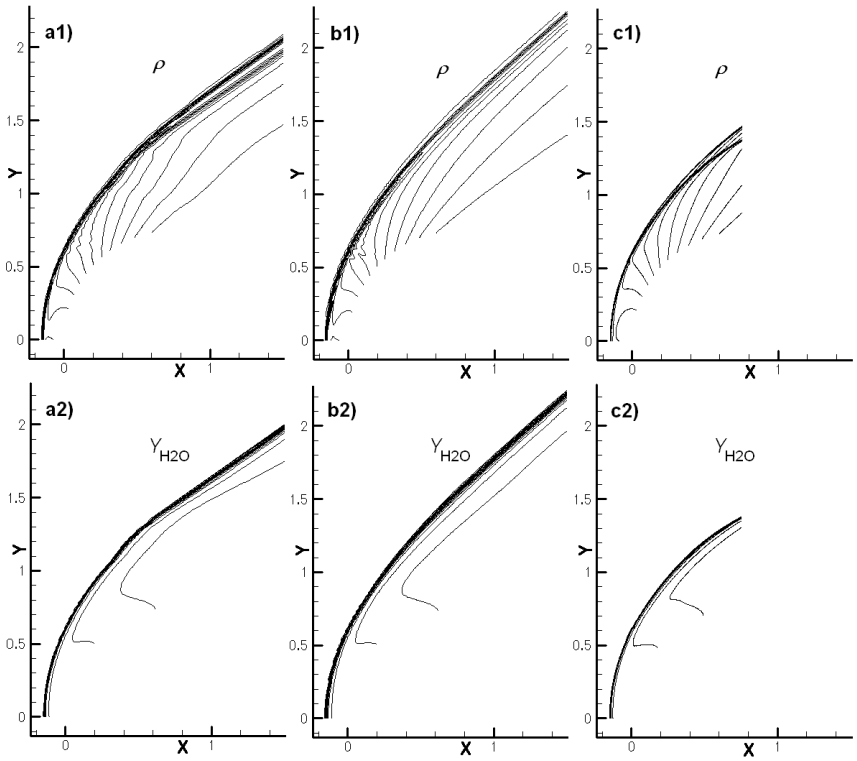

Figure 2. Property contours for the Eulerian formulation: a1) Grid 1 density contours; a2) Grid 1 H_2O mass fraction contours; b1) Grid 2 density contours; b2) Grid 2 H_2O mass fraction contours; c1) Grid 3 density contours; c2) Grid 3 H_2O mass fraction contours.

Figure 3 shows the position of the shock wave and the reaction front for the numerical solutions and for the experimental data. For the numerical solutions, in order to indicate the position of the fronts, two temperature contours were included. The difference in position of the oblique fronts for Grid 1 and Grid 2 evidences the influence of the format of the mesh. For Grid 1, for instante, the direction of the oblique reaction front is the same of the longitudinal faces of the cells. For Grid 3, despite the fact that the shock wave and the reaction front are dislocated upstream, and the distance between them is underpredicted, the positions of the oblique fronts compare better to the experimenal data. The effect of the mesh refinement is very similar to the one observed by Ess and Allen (2005). These authors simulated Lehr's experiment for Mach 6.46 using two meshes. In the coarse mesh, the shock and the reaction front remained visually attached. In the finer mesh, the detachment is barely observable.

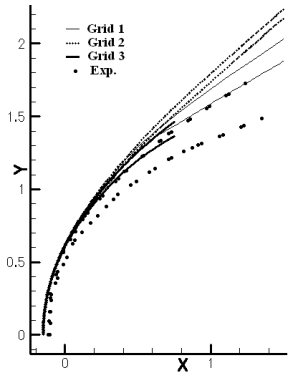

Figure 3. Position of the shock wave and reaction front. Comparisons to the experimental data (Lehr 1972).

3.2. Chemical Reaction Analysis 1

In Lehr's experiment for Mach number 6.46, as the fluid crosses the normal shock wave, the temperature increment is such that the induction time is reduced in a way that it is not possible to ditinguish the induction zone. As the shock wave becomes more oblique and the temperature increment diminishes, the induction time increases and the detonation wave distances from the shock wave. At a certain point, the temperature increment is not sufficient to ignite the mixture and the detonation wave progressively aligns to the local flow. Some control volumes in this region of the flow will inevitably be composed of gases with very different chemical compositions. In order to clarify the effect of using average species mass fraction for the condition of these volumes, simulations of chemical reaction under constant volume mode are carried out. Three initial chemical compositions are considered. For the first one, the initial mixture is composed of unreacted gas. For the second one, the mixture is composed of 99% of unreacted gas and 1% of reacted gas. For the third one, the mixture is composed of 95% of unreacted gas and 5% of reacted gas. Figure 4 shows the temperature evolution for the three simulations. The initial conditions are a stoichiometric H_2-air mixture, ρ = 0,002 g/cm^3 and internal energy such that T = 1200 K for the unreacted mixture. The small variation of the initial chemical composition reduced the induction time considerably. These simulations indicate that the use of average species mass fraction may have anticipated the oblique reaction front of the numerical solutions obtained with the Eulerian formulation, as presented in Figs. 2 and 3.

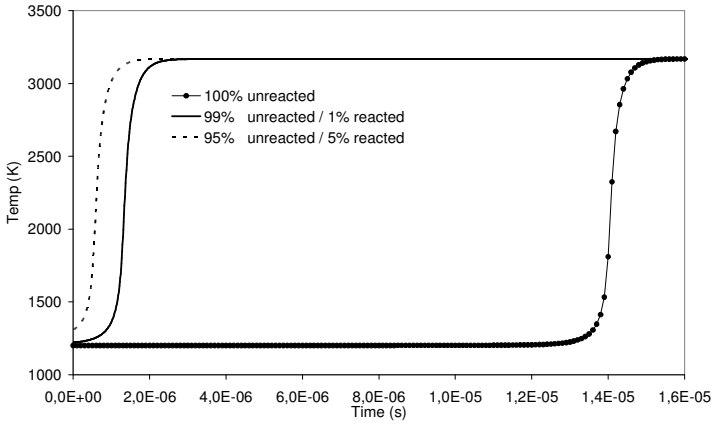

Figure 4. Temperature versus time for a chemical reaction under constant volume mode. Effects due to a small quantity of reacted gas in the initial mixture.

3.3. Wedge

Hypersonic flow around a wedge is simulated with the Eulerian and with the hybrid Eulerian/Lagrangian formulations. The freestream conditions are a stoichiometric H_2-air mixture, pressure equal to 0.266 atm, temperature equal to 300 K and Mach number equal to 7. The wedge semi-angle is equal to 35°. Simulations were carried out over two structured quadrilateral meshes. The meshes differ mainly in refinement. The boundaries of the meshes are presented in the Fig. 5. Grid 1 is composed of 34200 nodes and 33787 cells, in which the distribution is 114 × 300 points in the transversal and longitudinal directions, respectively. The nodes are equally spaced in each direction. Grid 2 is composed of 90000 nodes and 89251 cells, in which the distribution is 150 × 600 points. The nodes are also equally spaced in each direction. Position coordinates are in centimeters.

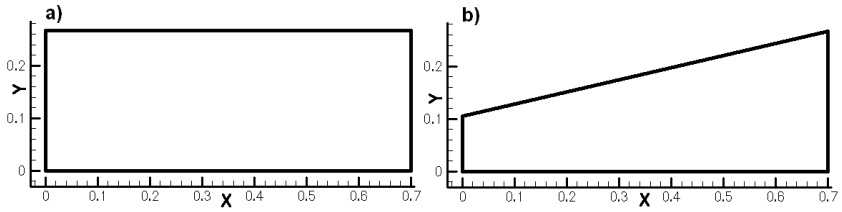

Figure 5. Boundaries of the meshes used to simulate the flow around a wedge: a) Coarse mesh (114 × 300), Grid 1; b) Fine mesh (150 × 600), Grid 2.

Figure 6 shows the density and the H_2O mass fraction contours of the solutions obtained. The overall structure of the flow is similar for all simulations. The distance that separates the shock wave to the detonation wave is progressively reduced up to the triple point and, then, the two fronts remain coupled downstream. Moreover, the same structure of the transition region, that exists between the initial oblique shock wave and the resulting oblique detonation wave, is observed for all solutions. The effect of the mesh is more significant for the Eulerian formulation, since the triple point is better defined for finer mesh.

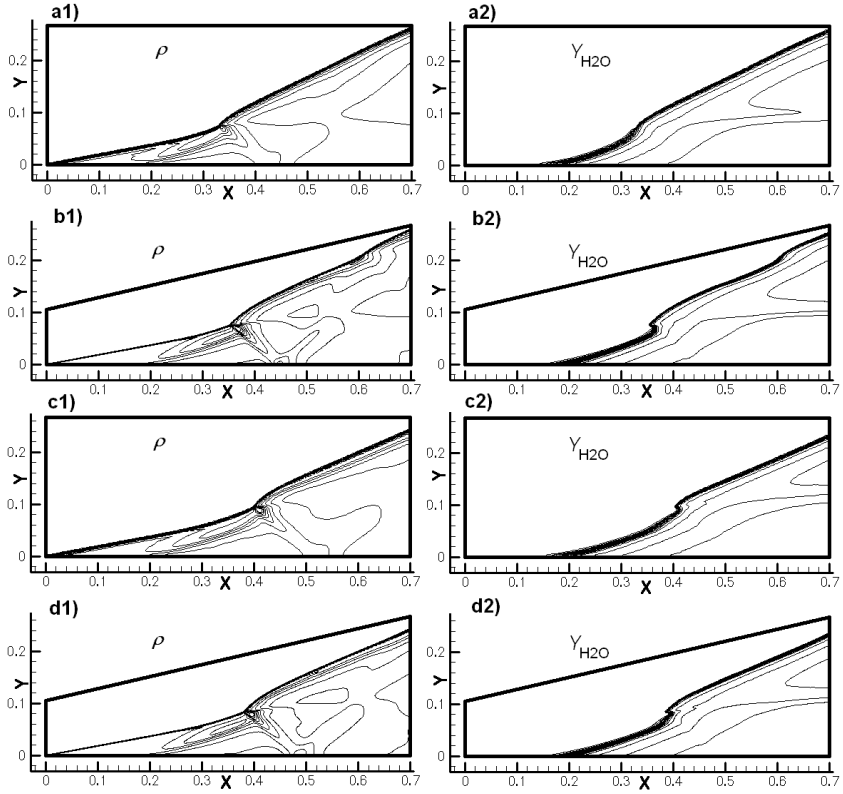

Figure 6. Property contours: Eulerian Formulation: a1) Grid 1 density contours; a2) Grid 1 H_2O mass fraction contours; b1) Grid 2 density contours; b2) Grid 2 H_2O mass fraction contours; Hybrid Formulation: c1) Grid 1 density contours; c2) Grid 1 H_2O mass fraction contours; d1) Grid 2 density contours; d2) Grid 2 H_2O mass fraction contours

Figure 7 shows the position of the shock wave and the reaction front for the solutions obtained. Two temperature contours are used to indicate the position of the fronts. Figure 7 a) presents the influence of the mesh refinement in the position of the two fronts for the Eulerian formulation, Fig. 7 b) presents the influence of the mesh refinement for the hybrid formulation, and Fig. 7 c) presents the influence of the formulation in the simulations performed for Grid 2. The effect of the mesh is more significant for the Eulerian formulation, since the reaction front as well as the triple point position move downstream with the grid refinement, as shown in Fig. 7 a). Such behavior is not observed for the hybrid formulation, Fig. 7 b). The position of the shock wave in the solutions obtained with Grid 2 is similar for the two formulations, as shown in Fig. 7 c), but the reaction front and the triple point position are dislocated upstream for the Eulerian formulation.

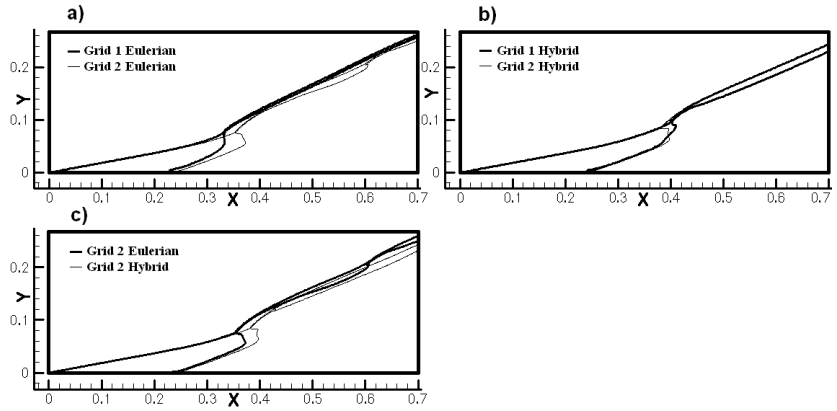

Figure 7. Position of the shock wave and reaction front: a) Comparison for the Eulerian formulation; b) Comparison for the hybrid formulation; c) Comparison between Eulerian and hybrid formulation for Grid 2.

3.4. Chemical Reaction Analysis 2

A second investigation of the reactive mixture is carried out to clarify the effects regarding the use of average species mass fraction in the induction zone. The previous analysis of the chemical reaction addressed the influence in the oblique reaction front that is approximately aligned to the local flow, in which some volumes may be composed of gases with very different chemical composition. The analysis of the present section addresses the reaction front approximately normal to the local flow. In this condition, the mixture of the control volumes in the induction zone is not composed of gases with very different chemical composition.

Simple one-dimensional simulations of chemical reactions under constant volume mode are carried out. The Eulerian mesh used is presented in Fig. 8. The density, energy and velocity are kept constant in space and time. The same conditions used in the analyses of section 3.2 are considered here. The freestream conditions consider unreacted stoichiometric H_2-air mixture, ρ = 0,002 g/cm^3 and T = 1200 K. The simulations are performed from the instant t_0 = 0 μs to the instant t_N = 20 μs. For a number of volumes equal to N, the time that a fluid takes to traverse a volume, Δt_{vol}, may written as

$$\Delta t_{vol} = \frac{t_N}{N} \cdot \tag{1}$$

For simplicity, two independent steps are considered, the first one for the fluid dynamics and the second one for the chemical reaction, in this order, *i.e.*,

$$\begin{aligned} \mathbf{Y}_i^{n+1/2} &= \mathbf{Y}_i^n + \left(\mathbf{Y}_{i-1}^n - \mathbf{Y}_i^n\right) \cdot \left(f_{\Delta t}\right), \\ \mathbf{Y}_i^{n+1} &= C\left(\mathbf{Y}_i^{n+1/2}, f_{\Delta t} \cdot \Delta t_{vol}\right), \end{aligned} \tag{2}$$

where C is the chemistry operator and $\mathbf{Y}$ is the vector of the chemical species mass fractions. $\mathbf{Y}$ is defined as

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ | \\ Y_M \end{bmatrix}. \tag{3}$$

$f_{\Delta t}$ is the time step divided by the time that the fluid remains within each cell, i.e.

$$f_{\Delta t} = \frac{\Delta t}{\Delta t_{vol}} \cdot \tag{4}$$

The numerical code VODE (Byrne and Dean, 1993) is adopted to time integrate the chemical composition from the instant t to the instant $t + \Delta t$.

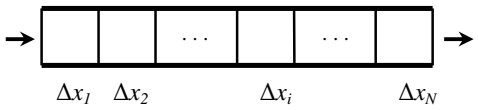

Figure 8. One-dimensional mesh used to simulate the time evolution of a reactive mixture under constant volume mode.

For the initial and the entrance boundary conditions, the freestream properties are defined for the overall volumes. The convergence is achieved when the maximum absolute variation of the temperature in a volume from the instant t to $t + \Delta t$ becomes lower than a certain tolerance. As initially, before the ignition, the variation of the temperature is insignificant, the convergence is only allowed when the maximum temperature variation becomes decrescent. Figure 9 presents the converged solutions for three meshes, the first one containing 20 cells, Fig. 9 a), the second one containing 100 cells, Figs. 9 b1) and b2), and the last one containing 1000 cells, Figs. 9 c1) and c2). Figures 9 b2) and 9 c2) are zooms of the Figs. 9 b1) and 9 c1), respectively. Six different time step values are considered, $f_{\Delta t}$ = 0.1, 0.3, 0.5, 0.7, 0.9 and 1.0. The simulation performed with $f_{\Delta t}$ equal to 1.0 corresponds to a simulation without considering average species mass fraction, since the integral information containing in a cell is passed to the following cell without mixing. The solutions presented in Fig. 9 have evidenced that the induction time is reduced when average species mass fraction is considered. This effect is minimized by the mesh refinement and by increasing the time step. These results and observations explain why the reaction front and the triple point moved downstream with the grid refinement for the Eulerian formulation in the simulation of a flow over a wedge, as shown in the Fig. 7 a). Moreover, such results also suggest that, even for the finer mesh, the distance from the detonation wave to the shock wave may have be underpredicted, as shown in the Fig. 7 c).

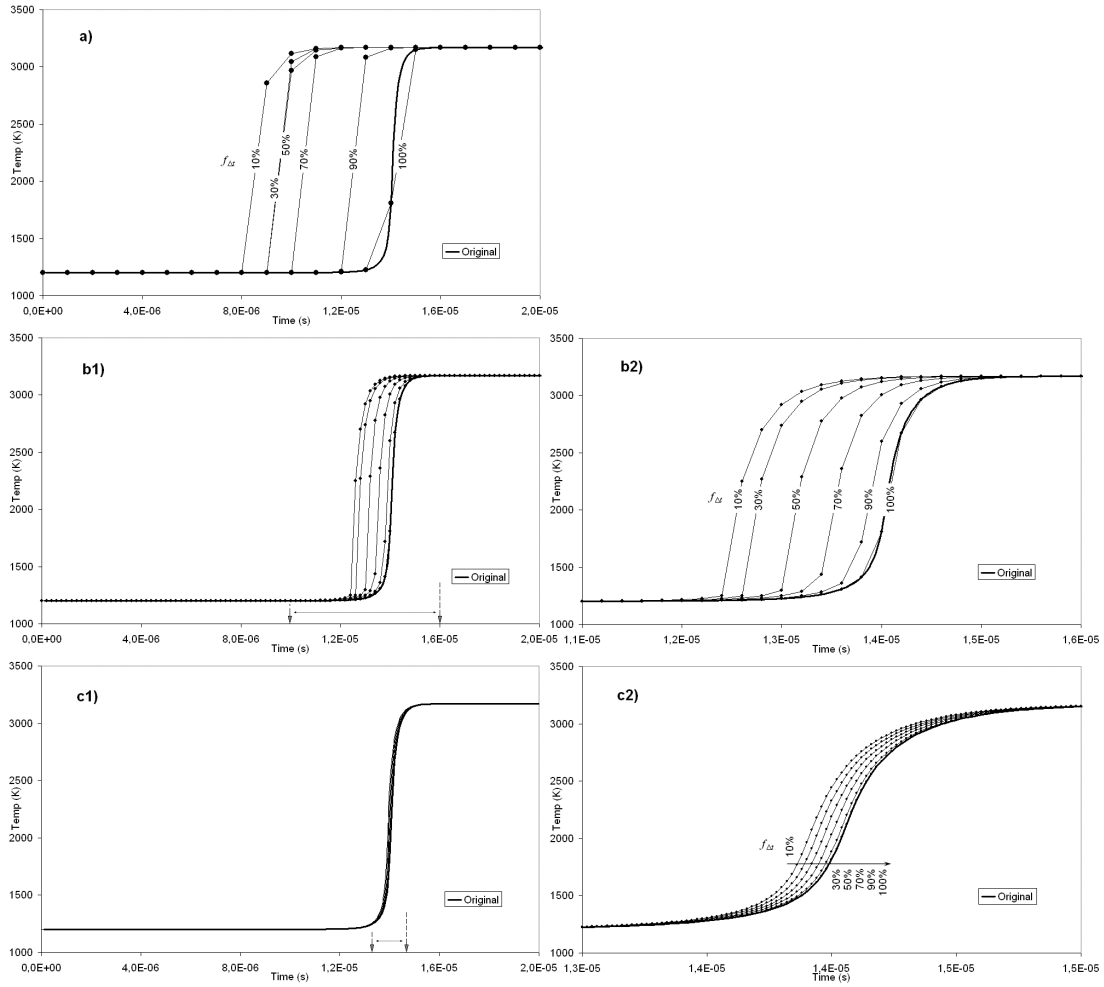

Figure 9. Effects of the use of the average species mass fraction. Comparison to the original time-evolving temperature profile: a) 20 cells, b1) and b2) 100 cells; c1) and c2) 1000 cells.

4. CONCLUDING REMARKS

Simulations of hypersonic reactive flows over a blunt body and over a wedge are performed using two different formulations to couple the chemical reaction to the fluid dynamics. The first coupling approach is achieved by Strang's time-step splitting procedure (Strang, 1968), and it was called an Eulerian formulation in the present paper. The second formulation uses particles that move with the fluid, and it was called a hybrid Eulerian/Lagrangian formulation. The description of this formulation is included in a companion paper also submitted to ENCIT-2008. For the simulations of hypersonic flow over a blunt body with the Eulerian formulation, the mesh format and refinement significantly influenced the final solution. For the simulations of hypersonic flow over a wedge with the Eulerian formulation, the distance from the reaction front to the shock wave was underpredicted. This effect is reduced with the refinement of the mesh. Similar observations of the influence of the grid refinement in the wedge simulation are noticed by Pimentel *et al*. (2002). The effect of the mesh format and refinement is considerably less significant for the hybrid formulation. Two independent investigations of the behavior of the reactive mixture showed that the use of average species mass fractions may reduce the induction time and shorten the induction zone. The second investigation also demonstrated that this effect may be minimized by mesh refinement and by increasing the time step.

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