Supplemental material for paper published in the International J of Hydrogen Energy, Vol. 30, 6044-6060, 2014. http://dx.doi.org/10.1016/j.ijhydene.2014.01.182

Application of a Laser Induced Fluorescence Model to the Numerical Simulation of Detonation Waves in Hydrogen-Oxygen-Diluent Mixtures

EULER CODE VALIDATION

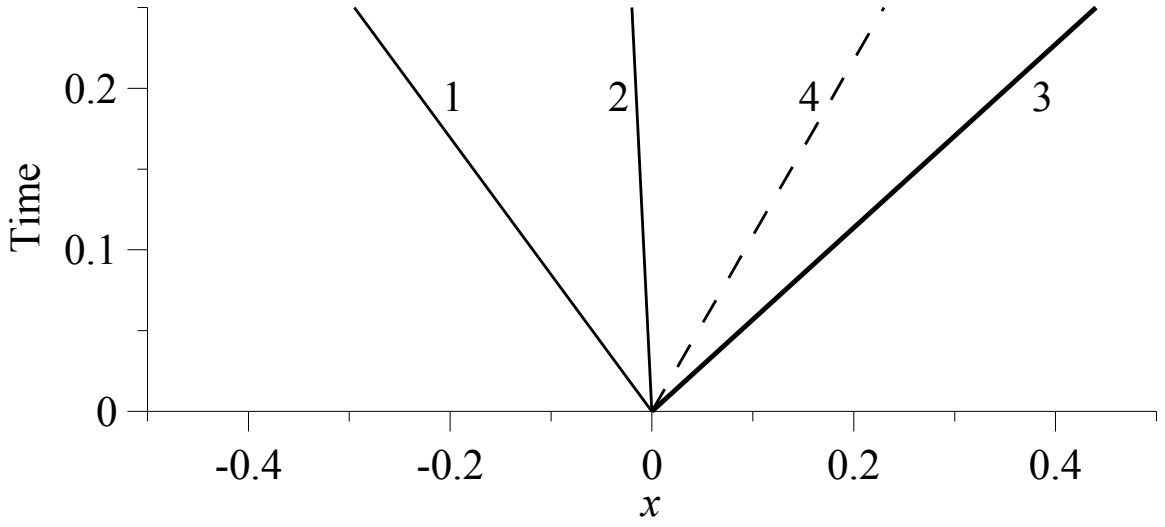
Introduction

Several test cases are presented in this section to demonstrate the accuracy and robustness of the Euler code used for simulations of cellular detonations. These test cases are logically divided in two groups: the first one deals with nonreacting flows of perfect gas and the second one with reacting flows, for which the thermochemical model used is the same as in detonation simulations. Each test case has specific objectives and the validity of the simulation results can be verified by comparison with a reference solution either obtained by the authors or known from the literature.
Unfortunately, direct comparisons of detonation simulations are not really possible because there is no real reference due to the instable nature of the numerical solution. In particular, it is not possible to validate a code by comparing a fluctuating numerical solution to a steady-state ZND solution. Instabilities exhibited by the detonation fronts in either 1D or 2D configurations are very sensitive to the intrinsic properties of the numerical schemes used. Hence, it is not sure that detonation simulation results obtained with one code are reproducible by another one except for some cases of very stable mixtures.

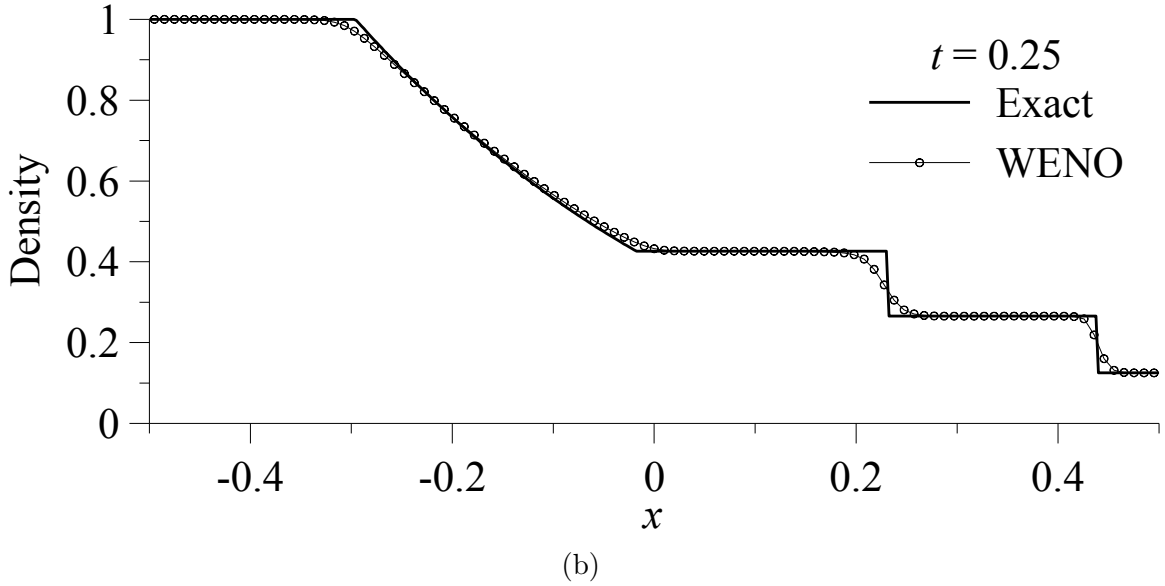
1D unsteady flow in a shock tube

This test case represents the classical 1D shock tube problem, which is used to test Euler solvers to see how they are able to resolve shocks, rarefactions and contact discontinuities. It belongs to the class of Riemann problems whose initial conditions ($t = 0$) are specified as two semi-infinite homogeneous states with a discontinuity at $x = 0$. The particular case presented below is the Sod problem, which is classically defined as follows. The gas is calorically perfect with a specific heat ratio of 1.4. The nondimensional parameters of the left sate are pressure 1 and density 1 whereas those of the right state are pressure 0.1 and density 0.125. The gas is initially at rest. At $t > 0$, the initial discontinuity is decomposed in three waves: a left-running rarefaction fan, and right-running shock and contact discontinuity; the latter separates the two states perturbed by the fan and shock. As the two initial states are homogeneous, the waves propagate at constant speeds and the flow states between them are constant. An exact selfsimilar solution can be obtained for this problem (see for example [1]).

The computational domain is 1D symmetric with respect to the coordinate origin, $x \in [-0.5, 0.5]$, with a uniform numerical grid of 101 points. The boundary conditions at both ends are treated as continuation or zero gradient. The exact wave front trajectories are plotted as a time-space diagram in Figure 1 (a). The exact and numerical solutions for the gas density at nondimensional time $t = 0.25$ are traced in Figure 1 (b). The rarefaction fan, delimited by the leading and trailing boundaries, produces a gradual density variation whereas the two other waves are marked by abrupt density changes. The numerical solution smoothes the flow parameter variation near the fan boundaries and at the discontinuities due to the dissipative properties of the numerical scheme, which guaranty stability and monotonicity of the solution. One can see that the wave velocities and intensities are well reproduced by the numerical result.



(a)



(b)

Figure 1: Sod problem solution: a) Exact wave trajectories in nondimensional time-space coordinates: 1: leading boundary of the rarefaction fan; 2: trailing boundary of the rarefaction fan; 3: shock; 4: contact discontinuity. b) Exact and WENO solutions for the nondimensional density at $t = 0.25$.

2D unsteady flow with a double Mach reflection

This test case is often used to validate Euler solvers by simulating an unsteady flowfield with strong shocks and triple points in 2D. The simulated flowfield can be experimentally obtained by installing a flat wedge in a shock tube. A normal shock, propagating at Mach number M_s, will interact with a wedge surface, which makes an angle α_s with the shock front as shown in Figure 2. This interaction results in a complex shock structure called a double Mach reflection that grows in time in a selfsimilar manner.

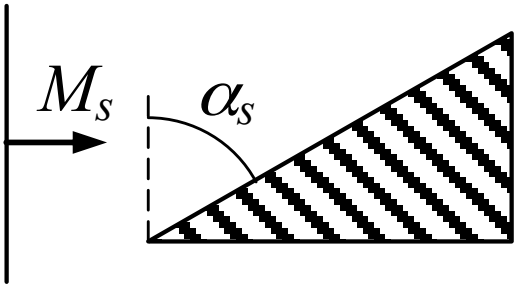


Figure 2: Schematic of a setup to generate a double Mach reflection.

To test our code, we took the numerical problem formulation from [2]. The computational domain is schematically shown in Figure 3. To simplify geometrical definition, the problem is considered in a Cartesian coordinate system whose x-axis is aligned with the wedge surface. The rectangular domain has dimensions $Lx \times Ly$. Figure 3 presents the initial condition when the shock front touches the wedge tip at point A. At this time instant, the straight shock front AB divides the domain in two zones with uniform gas states: the unperturbed state, Q_1, and the state behind the shock, Q_2.

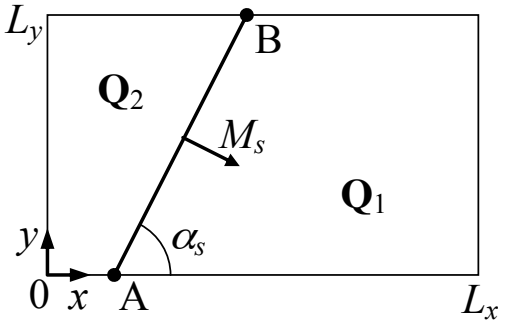
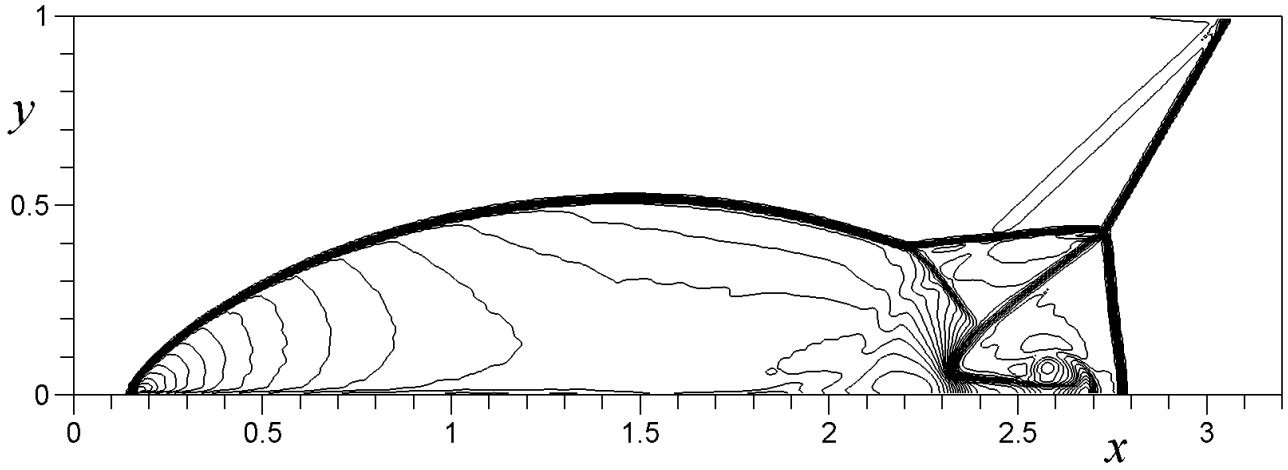
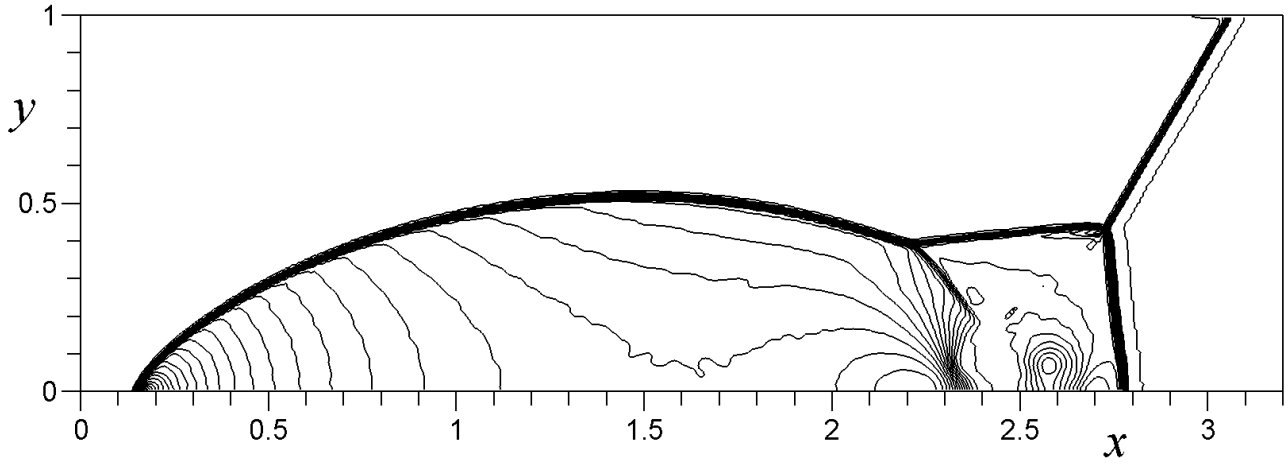


Figure 3: Schematic of the computational domain for simulating a double Mach reflection.

The boundary conditions are formulated as follows. State Q_2 is imposed on the left boundary. On the lower boundary, state Q_2 is imposed at $x \leq x_A$ and slip wall or symmetry conditions are used at $x > x_A$. On the upper boundary, states Q_2 and Q_1 are imposed on the left and right of point B respectively. On the right boundary, continuation or zero gradient conditions are used. During the simulation, the position of point A is fixed whereas point B moves along the upper boundary with the velocity corresponding to the normal shock propagation; this latter condition is valid if the gas state near the upper boundary remains unperturbed.
For the particular case presented below, the problem parameters were chosen as follows: $L_x = 3.2$, $L_y = 1$, $x_A = 1/6$, $\alpha_s = 60°$, $M_s = 10$. The gas is assumed to be calorically perfect with a constant



(a)



(b)

Figure 4: Instantaneous fields of density (a) and pressure (b) resulting from the double Mach reflection in nondimensional coordinates at $t = 0.2$. Number marks: 1: incident shock; 2: Mach stem; 3: first reflected shock; 4: contact discontinuity; 5: curved shock; 6: second reflected shock; 7: jet head.

specific heat ratio of 1.4. Nondimensional flow parameters that characterize state Q_1 are density 1.4, pressure 1, velocity magnitude 0, and sound speed 1. Given a nondimensional shock speed of 10, flow parameters corresponding to state Q_2 are density 8, pressure 116.5, velocity magnitude 8.25, and sound speed $\approx$4.515. The computational mesh is Cartesian with a uniform step of 1/120 in both directions. The time advancement is controlled by a Courant number ≤ 0.7.

The computational result at nondimensional time $t = 0.2$ is given in Figure 4. The pattern of the first Mach reflection is composed of the incident and reflected shocks on the upper side and a Mach stem near the wall. This creates two gas flows separated by a strong contact discontinuity. The second Mach reflection pattern has the inverse orientation and results from the intersection of the first reflected shock and the curved shock originating from the wedge tip. As a result, a second reflected shock is formed as well as a weak contact discontinuity, which is not visible in the density field. The pressure behind the Mach stem is lower than that between the wall and the curved shock. This longitudinal pressure gradient drives a jet flow near the wall. One can compare the present results with those shown in Figure 4 of [1] in order to see that the flowfields computed with different codes are very similar including the shock front positions and the contour line patterns.

Selfignition in a closed volume

This test case is intended to validate the numerical integration scheme and to check its capability to treat stiff problems with chemical source terms. The problem is equivalent to a homogeneous constant volume reactor, for which a reference solution can be obtained using 0D models with stiff ODE solvers like, for example, SENKIN [3] of the CHEMKIN-II package [4].

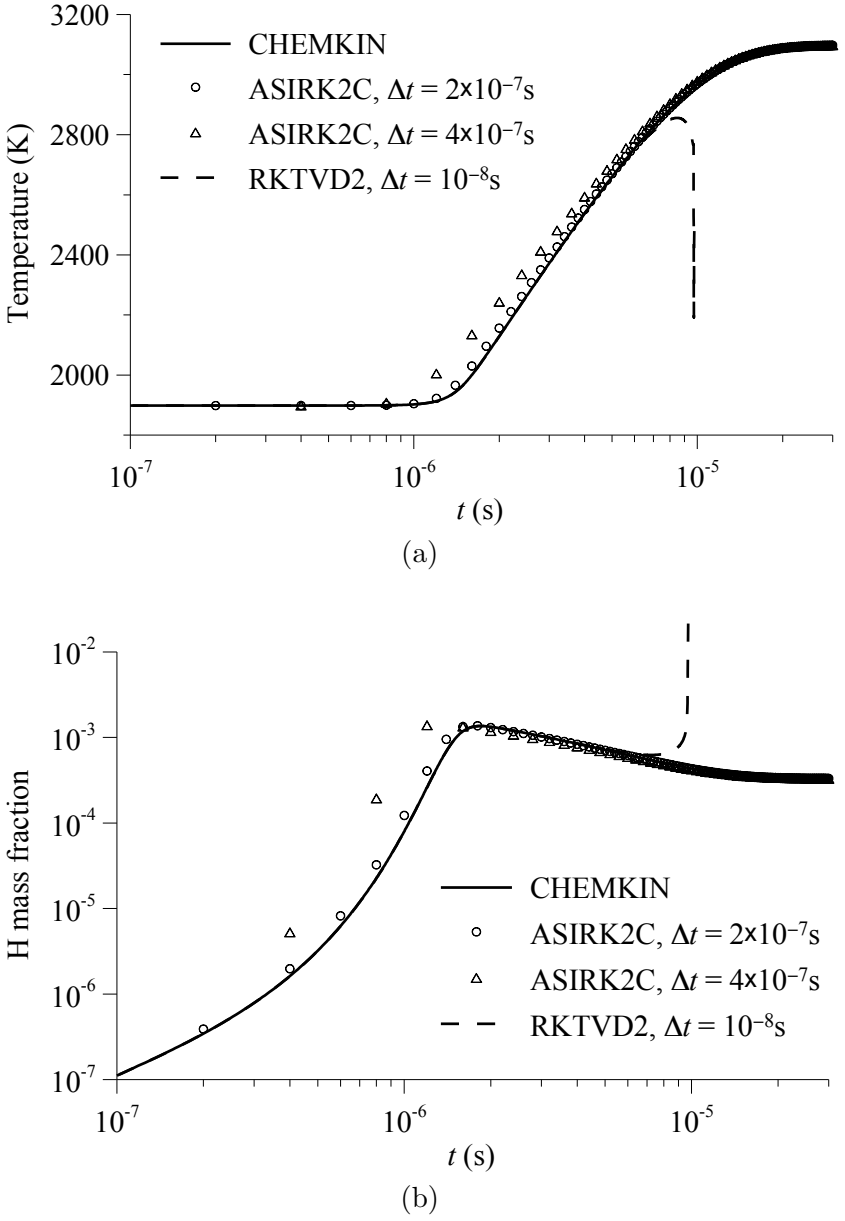


Figure 5: Temporal profiles of temperature (a) and H radical mass fraction (b) in a constant volume reactor obtained using CHEMKIN and the Euler code with different integration schemes and time steps.

A square computational domain is considered with the symmetry boundary conditions. The geometrical dimensions are chosen large enough to avoid any time step limitation by the CFL stability condition. The mesh is simply 3 by 3 points. To be representative with respect to the detonation simulations considered below, we took a H_2-O_2 stoichiometric mixture diluted with Ar in a volumetric proportion 1/4. The mixture is at rest, its initial pressure and temperature correspond to the post-

shock conditions of a Chapman-Jouguet detonation: 0.4994 MPa and 1898 K.

Numerical results for this problem have been obtained with two second-order Runge-Kutta integration schemes available in the Euler code: the RKTVD2 explicit scheme with TVD properties and the ACIRK2C semi-implicit scheme whose explicit part is identical to RKTVD2. The time step was fixed during all the integration process. These results are compared with a reference solution produced by the SENKIN code of CHEMKIN-II in Figure 5. One can see from this comparison that the ACIRK2C scheme provides stable solutions even if integration errors are significant due to a large time step. With time reduction, the solution converges to the reference one. On the contrary, solutions produced by the RKTVD2 scheme with a much smaller time step coincide with the reference solution during some part of the combustion process but become instable when approaching the chemical equilibrium. This test clearly proves the robustness of the ACIRK2C scheme and the advantage that it has in reactive simulations.

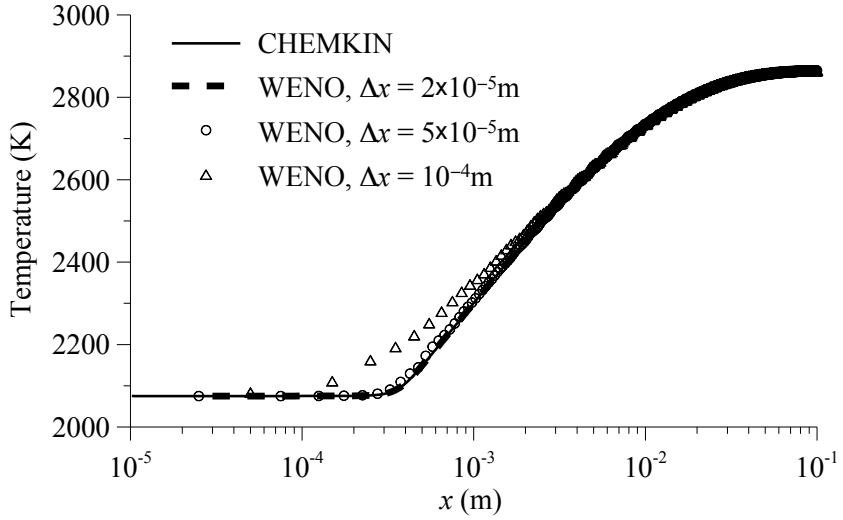
Selfignition in a 1D steady flow

This test case is to verify the spatial resolution of a reaction front by the WENO scheme of the Euler solver. The problem corresponds to a constant area tube with a hot flow of fresh mixture at the entrance. If the flow velocity is sufficiently high, the diffusion effects in the reaction zone can be neglected. A steady-state problem of this kind is described by a set of ODE that can be numerically integrated along the spatial coordinate to get a reference solution.

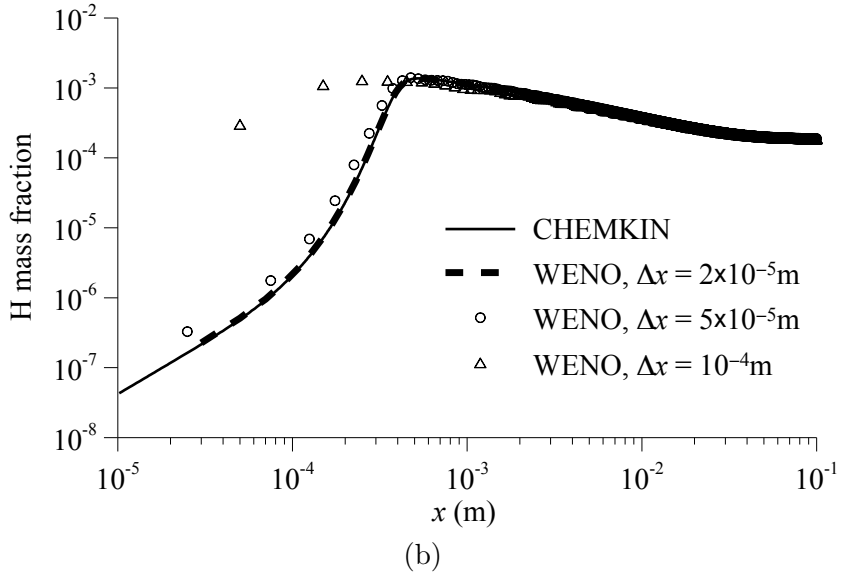
The length of the computational domain is $L = 0.1$ m. A 1D mesh is defined by two parameters: the length of the first part with a constant step, L_1, and the corresponding step, Δ_{x1}. In the second part of the mesh, the step is progressively increasing. Three 1D meshes, composed of 1000 points, were used: (i) $L_1 = L$, $\Delta_{x1} = 10^{?4}$ m; (ii) $L1 = L/4$, $\Delta_{x1} = 5x10^{?5}$ m; (iii) $L1 = L/10$, $\Delta_{x1} = 2x10^{?5}$ m.

Characteristic boundary conditions were used at both ends of the domain allowing to deal with the subsonic flow. To be representative, we took as a reference solution a part of a ZND solution for an overdriven detonation starting from the post-shock state. The gas is initially composed of a H_2-O_2 stoichiometric mixture diluted with Ar in a volumetric proportion 1/4. The detonation velocity is 1600 m/s in comparison to the Chapman-Jouguet velocity of 1518 m/s. Due to the overdriven regime, the final Mach number of the combustion product flow is 0.7 and the numerical solution can be stabilized whereas it is always instable in the Chapman-Jouguet regime with a choked flow. The theoretical inlet state is defined by pressure 0.5556 MPa, temperature 2075 K and flow speed 405.1 m/s; the corresponding final state is defined by pressure 0.4264 MPa, temperature 2866 K and flow speed 693.5 m/s.

Numerical results provided by the Euler code on different meshes are compared with a reference solution, produced by a ZND code based on CHEMKIN-II, in Figure 6. Numerical solutions obtained on the two finer meshes are in good agreement with the reference one. On the coarsest mesh, the induction distance is significantly reduced due to numerical errors. One can note an important fraction of the H radical in the very first mesh point. The solution being sensitive to the numerical errors is not fully steady in this case and exhibits periodical fluctuations, which disappear after mesh refinement.



(a)



(b)

Figure 6: Spatial profiles of temperature (a) and H radical mass fraction (b) in a 1D reacting flow obtained using a CHEMKIN-based ZND code and the Euler code with different meshes.

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