SECONDARY DETONATION CELLS IN SYSTEMS WITH HIGH ACTIVATION ENERGY

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Experimental studies of gaseous detonations (see, for example, [1,2]) and multidimensional numerical simulations of the detonations using a one-step Arrhenius kinetics [3] have shown that an increase in activation energy leads to more irregular cellular structures. The experiments also indicate that small secondary cells can appear inside the main structure when the activation energy is high enough [1,2]. An analysis [4,5] of similar phenomena in liquid explosives has shown that the secondary cells may occur when the overdriven parts of the cellular detonation front become unstable enough to form secondary triple points during the time between two collisions of the primary triple-shock configurations. Secondary triple points have been reported in numerical simulations [3], however, the activation energy and numerical resolution were not high enough to obtain well formed secondary cells. In the present work, we consider a reactive system with a high activation energy, and use adaptive mesh refinement to resolve the secondary triple points.

The reactive system is described by the polytropic equation of state and a one-step Arrhenius kinetics. The complete thermodynamic definition of the system is given in [3]. The thermodynamic parameters of the system (the polytropic exponent $\gamma = 1.333$, the heat of chemical reaction $Q = 4.867$ MJ/kg, the initial density $\rho_0 = 0.493$ kg/m^3 and the molecular weight $M = 0.012$ kg/mol) approximately correspond to the stoichiometric gas mixture $2H_2 + O_2$ at $P_0 = 1$ bar, $T_0 = 293$ K. We used the activation energy $\mathrm{E}_a = 35$ kcal/mol (or $\mathrm{E}_a/\mathrm{RT}_* = 10.3$, or $\mathrm{E}_a/\mathrm{RT}_0 = 60$, where $\mathrm{T}_* = 1709$ K is the controlling temperature behind the leading shock front moving with the Chapman-Jouguet (CJ) velocity, and $\mathrm{T}_0 = 293$ K is the temperature in the initial state). The pre-exponential factor $A = 4.5 \times 10^{10}$ s^{-1} corresponds to 0.054 mm for the half-reaction zone length of CJ detonation.

The reactive Euler equations were solved on a structured mesh using an Eulerian, Godunov-type numerical scheme incorporating a Riemann solver. An adaptive mesh refinement algorithm based on the Fully Threaded Tree (FTT) [6] and extensively tested in reactive fluid dynamic simulations (see, for example, [7]) was used to increase the resolution locally as required by the changing physical conditions. The minimum computational cell size was 6.3×10^{-4} mm which is of the order of the viscous scale. Further increase of the numerical resolution would require solving the Navier-Stokes equations.

The model was tested for the case $\mathrm{E}_a = 25$ kcal/mol ($\mathrm{E}_a/\mathrm{RT}_* = 7.4$ or $\mathrm{E}_a/\mathrm{RT}_0 = 43$) described in [3]. The test calculations show that the numerical technique used in the present work and the FCT-based technique used in [3] give basically the same results for the same resolution (approximately 7 computational cells per half-reaction zone length). The FTT-based calculations with 10 times higher resolution in the region of energy release show very fine details in the structure and dynamics of the cellular detonation front. In particular, we see the vorticity generation along the slip lines behind the triple points and the amplification of the vorticity during the interactions of the transverse waves with unreacted pockets. However, even at this high resolution, there is no well formed secondary cell structure.

For $\mathrm{E}_a = 35$ kcal/mol, we used 7 levels of mesh refinement and achieved the resolution of 86 computational cells per half-reaction zone length. The temperature field in Fig. 1 shows the multiple secondary triple points that appear between two primary triple-shock configurations as a result of instability of the overdriven parts of the detonation front. The secondary triple points form the small detonation cells which grow as the overdrive decreases. These small cells disappear in the middle of the primary cell when the secondary transverse shocks can no longer cause enough energy release in the induction zone.

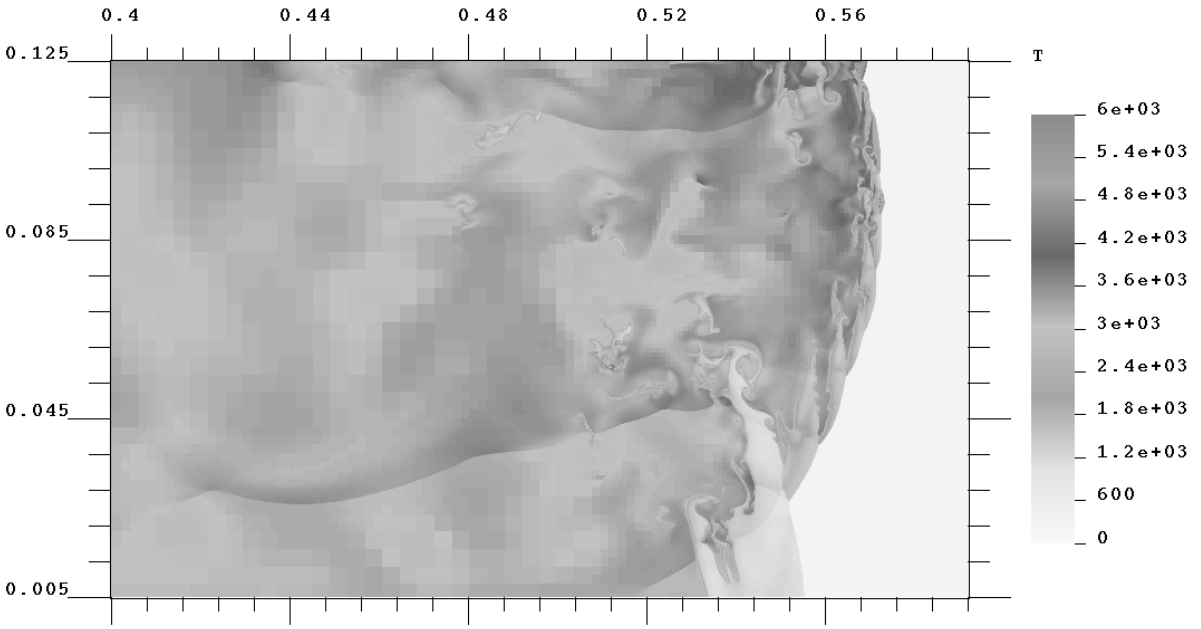

Fig. 1. Temperature field (K) behind the cellular detonation front for $E_a/RT_* = 10.3$. The horizontal and vertical scales are in centimeters.

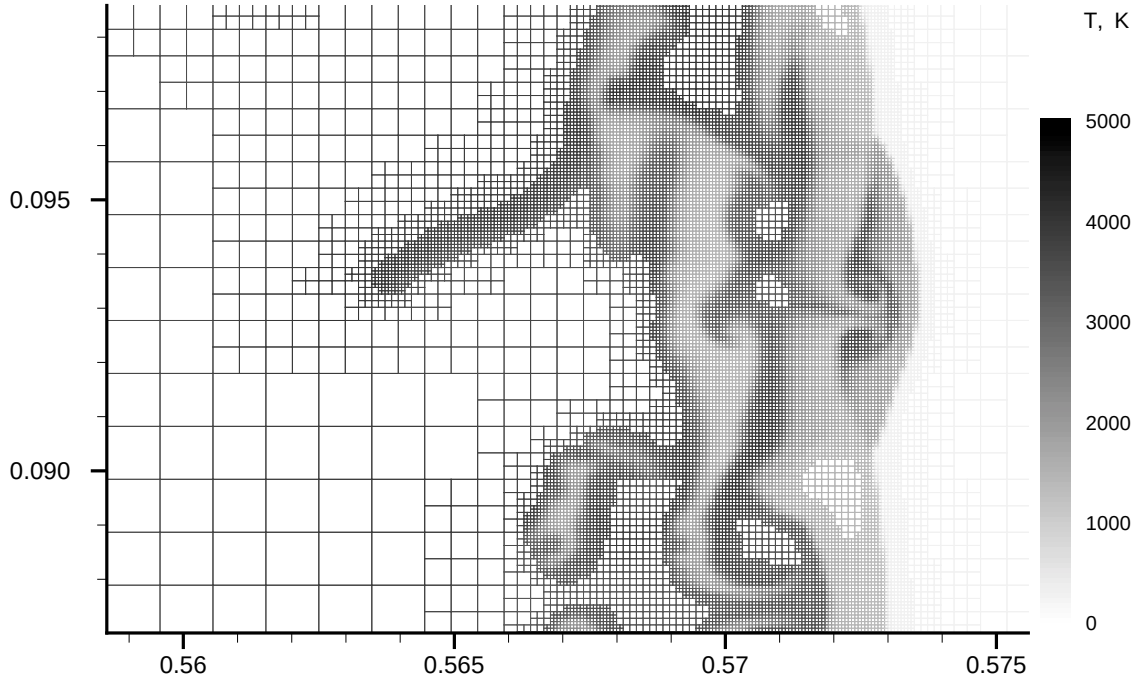

Fig. 2. Computational mesh for a small fragment of Fig. 1. The gray scale shows the temperature field.

A part of the secondary structure of the detonation front is presented in Fig. 2, which shows the temperature field and the computational mesh for a small fragment of Fig. 1. The fine mesh covers the regions with increased gradients and allows us to resolve the details of the secondary structure including the triple points, transverse shocks, induction zones, unreacted pockets, and vortical structures in the reactive flow.

The present work is the first numerical study of the secondary detonation cells in systems with high activation energy. It confirms that the secondary cellular structure can exist in reactive systems with a one-step Arrhenius kinetics of energy release. The results presented here are in qualitative agreement with the experimental observations [1] which indicate that the secondary cellular structure appears when $E_a/RT_* > 6.5$.

References.

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