Multi-Headed Detonations in Oxygen-Aluminum Mixtures: Two-Dimensional Numerical Simulations Using Adaptive Grid Refinement

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Introduction

The study on the detonation wave propagation in multi-phase mixtures is of special importance due to the dust explosion hazards seen in the contemporary industry. Specifically aluminum is a commonly used material, both in production and e.g., as a component of solid rocket propellants. This energetic material, if used in the form of fine particles, has strong ability to ignite and combust. After transition to the detonation it can show its highly destructive power.

In this paper the numerical studies on the detonations in multi-phase mixtures are presented.

Problem Formulation

In this paper the propagation of the detonation in oxygen-aluminum particles, two-phase mixture is studied numerically. Two-dimensional case is considered. The mixture is modeled using the continuum mixture theory; i.e., fine solid particles suspended in the multi-component gas mixture are treated as the continuum. Both continua can be in thermal and mechanical non-equilibrium. Although the particles are assumed small, spherical, non-compressible and non-interacting with each other, their volume is not neglected. Such assumption, although very common does not simplify significantly the system of equations and is not needed. It is also difficult to find reasonable criteria when this factor is negligible and when it is not. The viscous, diffusion and heat conduction terms are neglected. The gas phase obeys the thermally perfect equation of state. Similarly, the solid phase internal energy and specific heat are also temperature-dependent. The phase interactions are described as the mass, momentum and energy exchange terms, and included in the equations in the form of the source terms. The full system of equations can be obtained by simple extension of the one-dimensional version presented elsewhere (see e.g., Benkiewicz et al. [1]).

The mass transfer (solid phase burning) is calculated based on the formula used by Borisov et al. [2], but due to the multi-component nature of the gas mixture, the combustion model is slightly more complicated than in [2]. In this research it is assumed that the burning rate taken from [2] describes the solid/liquid aluminum consumption rate. The gas phase can contain O_2, AlO, and Al_2O_3. Although Al_2O_3 generally does not exist in gas phase it is assumed that it can be present in the form of very fine particles that behave as a gas and are treated as a gaseous

component. It can contribute to the gas phase internal energy and specific heat, but due to the lack of transport data it does not contribute to the gas phase viscosity and heat conduction coefficients. It is also assumed that the aluminum combustion product is Al_2O_3, but if the gas phase exceeds the limiting value of $T_{decomp}=3500$ [K] then the aluminum is burnt into AlO, and Al_2O_3 starts to decompose into AlO and O_2.

Computational Technique

The set of equations is solved using the Adaptive Mesh Refinement (AMR) technique proposed by Berger et al. [3]. In this approach one coarse grid and the set of hierarchical grid layers (patches) with increasing spatial resolution is used in order to improve the precision in the most interesting areas of the flow such as shocks, contact discontinuities, solid phase interfaces, high gradients, etc. This set of grid patches is self-adopting to the flow conditions; i.e., the grids are automatically placed and removed in the most interesting parts of the flow field.

The Adaptive Grid Refinement and the integration procedure are very independent on each other. Specifically in the AMRCLAW package Berger et al. [4] applied the time splitting technique and Godunov-type interleaving of PDE and ODE solvers. For the purpose of this research the homogeneous part of the system of equations (PDE) is solved using the Godunov-type unsplit MUSCL-Hancock TVD numerical method with HLLE approximate Riemann solver for the gas phase (see Toro [5]) and a “good” approximate Riemann solver for the solid phase (see Benkiewicz et al. [1]). The source terms (ODE) is integrated using the highly accurate VODE subroutine from the CHEMKIN-II package.

Results

The case considered here is the propagation of the detonation in the long channel. The solution of the one-dimensional case is used as the initial state for the two-dimensional computations. Some of the initial conditions are summarized in Table 1.

Solid phase concentration [kg/m^3]:	0.4
Particle diameter [μm]:	5.0
Domain size (length x height) [m]:	1.6 x 0.16
Coarse grid size:	200 x 20
Refinement levels (ratios):	2 (4/4)
Equivalent uniformly fine grid size:	3200 x 320

Table 1. Initial conditions.

Figure 1 presents the pressure distribution at the initial stage of the development of the detonation at *t=0.50-0.62* [ms] (frames taken every *0.02* [ms]). The pictures cover the right end of the computational domain. The sequence clearly shows the dynamics and unsteadiness of the detonation front. In Fig. 1-(a) two triple points that can be identified by high-pressure regions, approach each other. One can easily find the incident and reflected shocks, and Mach stems. In Figs. 1-(b) and (c) the collision of triple points in the central part of the channel leads to local

explosion and the high-pressure region. This collision point later becomes the new Mach stem and the source of the new triple points. One can also find weaker waves and triple points reflected from the walls. The Mach stems seen in Fig. 1-(a) now become the incident shocks and the triple points now transverse towards the walls. In Fig. 1-(e) they collide with the triple points reflected from the walls. Two new local explosion centers lead to generation of new Mach stems and new triple points. This process will be repeated several times leading to the multi-headed detonation. Since the results shown in Fig. 1 cover only the initial and transient process, it is very difficult to predict if the detonation propagates as the two-headed structure. This problem will require further investigation.

Figure 2 shows the comparison of the various parameters at the detonation front at *t=0.62* [ms]. The frames present pressure, gas temperature, logarithm of the solid phase concentration (better resolution of the differences) and the mass fractions of Al_2O_3, AlO and O_2, respectively. The flow field structure suggests that the propagating waves surround pockets of unburned fuel. These pockets are burned later, quite far behind the detonation front leading to very non-uniform species distribution.

Conclusions

The computer simulations of the detonation in the mixture consisting of the oxygen and aluminum particles have been performed using the Adaptive Mesh Refinement combined with the high-order, contemporary numerical methods. The AMR technique leads to precise solution of the detonation front. The computations show the development of the triple points, incident shocks, Mach stems, local explosion centers, and finally the transition into the multi-headed detonation. It is probably the first time when the detailed structure of the detonation front in the oxygen-aluminum mixture has been obtained in numerical simulations.

References

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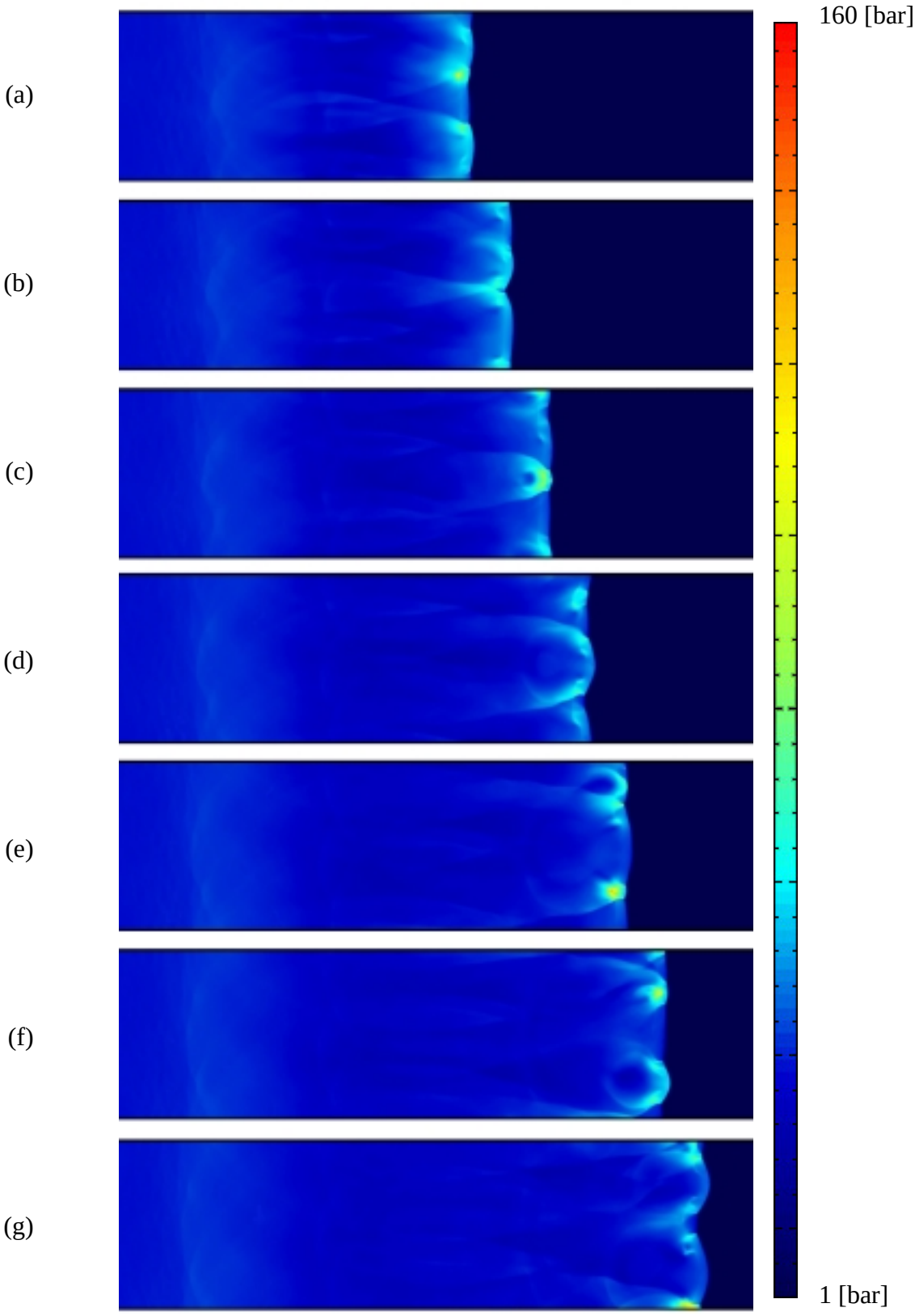

Fig. 1. Pressure distribution at *t=0.50-0.62* [ms].

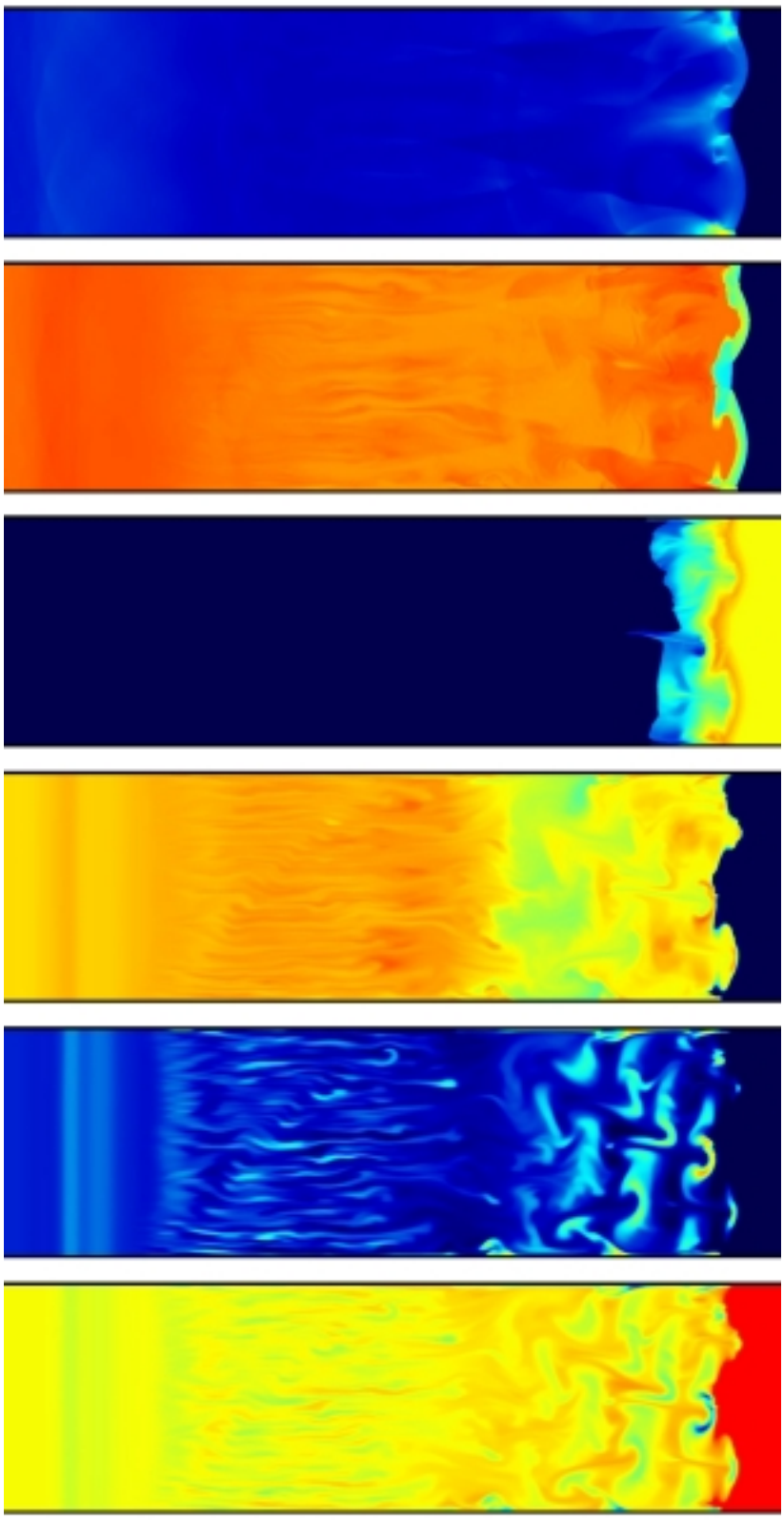

Fig. 2. Comparison of pressure, gas temperature, logarithm of the solid phase concentration, and species mass fractions at *t=0.62* [ms].