EFFECTS OF BOUNDARY LAYERS ON SHOCK-FLAME INTERACTIONS AND DDT

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Abstract. The effects of boundary layers on shock-flame interactions and deflagration-to-detonation transition (DDT) are investigated using two- and three-dimensional, time-dependent, reactive Navier-Stokes fluid-dynamics simulations of shock-tube experiments [1,2]. A dynamically adapting mesh is used to resolve flames, shocks, boundary layers, and vortices in flow. Simulations show a complex sequence of events, starting from the interactions of an incident shock with an initially laminar flame and the formation of a flame brush. The bifurcation of the reflected shock, due to boundary layer effects, creates a complex structure containing a rapidly growing, leading oblique shock followed by a recirculation region. If the flame is initially close enough to the bifurcated structure, it becomes entrained in the recirculation region and attached to the bifurcated shock. Three-dimensional simulations show that the highly deformed flame surface is spread out through the entire region between the reflected shock and the end wall. The schlieren pictures made from three-dimensional data show a reflected shock followed by a region of approximately constant-volume burning. The burning region moves with the velocity of the reflected shock and is characterized by the pressure that is less than the pressure of a Chapman-Jouguet (CJ) detonation. A reactive bifurcated structure affects the flow both qualitatively and quantitatively. It increases the energy-release rate in the system, leads to the formation of Mach stems in the middle of the shock tube, and generates multiple hot spots behind the Mach stem, thus facilitating DDT. The DDT process finally leads to the emergence of a self-sustained cellular detonation.

Introduction. The interactions of reflected shocks with a flame have been used to study flame instabilities and development of turbulent flames [3], shock amplification [4], and DDT [1,2]. Recent numerical simulations [5,6] reproduced both shock amplification and DDT seen in the experiments. However, some experimental features were not reproduced adequately. Among these was the presence of a "strange" combustion wave moving behind or with the reflected shock at approximately half of the CJ detonation velocity and considerably lower pressure [1,2]. Simulations [5,6] modeled a shock-flame interaction in the middle of a shock tube and did not include the effects of boundary layers. Here we describe new simulations that include these effects in conditions corresponding to [2]. New simulations show the strange combustion wave, and give an explanation of its structure and how it originates.

Model. We consider a stoichiometric ethylene-air mixture at the initial pressure $P_0 =$ 100 Torr and the initial temperature $T_0 = 293$ K. The reactive system is described by the time-dependent, compressible, reactive Navier-Stokes equations which include the effects

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of thermal conduction, diffusion, shear viscosity, and chemical reactions, similar to [5,6]. The equations are solved using a fully threaded tree (FTT) adaptive mesh refinement, second-order, Godunov-type fluid dynamics code [7]. The equation of state is that of an ideal gas, $P = \rho RT/M$, $E = P/(\gamma - 1)$ where R, $M = 29$ g/mol, and $\gamma = 1.15$ are the gas constant, molecular weight, and adiabatic index, respectively. The chemical source term describes first-order Arrhenius kinetics, $\dot{Y} = -A\rho Y \exp(-Q/RT)$, where Y is the mole fraction of the reactant, $A = 3.2 \times 10^{11}$ m^3/kg-s, and $Q = 30.74RT_0$. Taking $\dot{Y}$ proportional to ρ accounts for the binary nature of chemical reactions taking place in real combustion systems. A similar temperature dependence is assumed for the kinematic viscosity $\nu = \nu_0 T^n/\rho$, diffusion, $D = D_0 T^n/\rho$, and heat conduction, $K/\rho C_p = \kappa_0 T^n/\rho$, where $\nu_0 = D_0 = \kappa_0 = 7.0 \times 10^{-6}$ g/s-cm-K^n are constants, $C_p = \gamma R/M(\gamma - 1)$ is the specific heat at constant pressure, and $n = 0.7$ models the temperature dependence typical of these coefficients in reactive hydrocarbon systems. The system parameters were selected to reproduce the experimentally measured laminar-flame speed and thickness, the Chapman-Jouguet (CJ) detonation velocity, the detonation-wave thickness, and their behavior as a function of temperature and pressure.

In two-dimensional computations, we simulate a 22.8 cm by 3.8 cm section of the shock-tube [2], and use reflecting, no-slip boundary conditions on the right and bottom, a zero-gradient inflow boundary on the left, and symmetry (mirror) conditions on the upper boundary. We thus model half of a cylindrically expanding flame (Figure 1). Three-dimensional computations simulated the corresponding 22.8 cm by 3.8 cm by 1.9 cm section of the tube and a quarter of a spherically expanding flame. The flame has an initial radius of 3.3 cm, and its center is 11.7 cm from the end wall. An incident shock is placed 0.4 cm in front of the flame surface. The velocity of the gas is set to zero everywhere ahead of the shock. Between the left boundary and the shock, the flow is uniform with the post-shock parameters determined from the Rankine-Hugoniot conditions for a shock with a given Mach number, M_s.

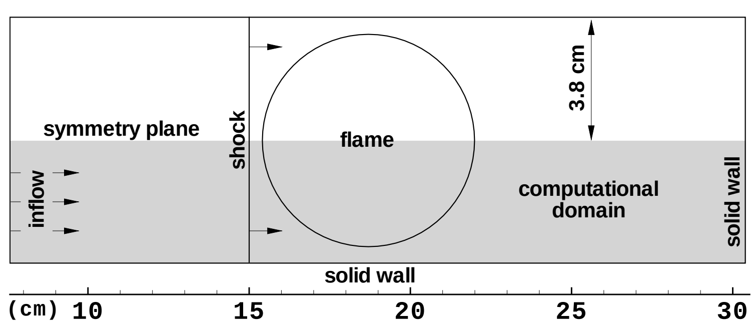

Figure 1. Two-dimensional computational setup.

Computations. An overall picture of the development of the flow for $M_s = 1.9$ is shown in Figure 2. An incident shock **I** interacts with the flame **F** and distorts it. Transmitted shock then reflects from the end-wall, the reflected shock **R2** passes through the flame and further distorts it. Richtmyer-Meshkov (RM) instability caused by the shocks creates funnels of unreacted material, **J1** and **J2**, which penetrate the flame. Interaction of primary shocks with the flame creates secondary shocks, pressure and rarefaction waves moving in all directions. Vorticity is generated continually during shock-flame interactions through small-scale RM and Kelvin-Helmholtz instabilities that further perturb the flame surface. All these interactions eventually transform the smooth flame surface into a highly disturbed turbulent flame brush. Secondary shocks absorb the energy of combustion, eventually overtake and strengthen **R2**.

By 342 μs, **R2** has passed through the flame, and a strong bifurcated structure **B3** begins to develop due to boundary-layer effects. As the bifurcated foot forms, a recirculation region appears behind it. The flame, which almost touches the bottom wall, penetrates the recirculation region, and then quickly spreads inside the recirculation zone. The energy released by the flame in the recirculation region accelerates the growth of the bifurcated foot until the foot reaches the symmetry plane and forms a Mach reflection at the top boundary. The energy release gradually increases the strength of the bifurcated shock and Mach stem. Eventually, the temperature behind the Mach stem becomes high enough to ignite the mixture. The ignition produces several hot spots, spontaneous waves, and residual flames that grow quickly, interact with vortices, and eventually trigger a detonation. The detonation wave propagates in all directions, consuming the high-density unreacted material in the funnel and behind the oblique shock. When the detonation enters the relatively low-density unreacted material compressed only by the incident shock, it forms the transverse-wave structure that creates detonation cells.

Figure 3 shows the main reflected shock and the surface of the flame at 457 microseconds in a three-dimensional simulation with $M_s = 1.6$. The flame has penetrated the recirculation regions behind the shock and is trailing behind with approximately the speed of the shock. The unburned material entering the shock is deflected to the middle of the tube where it flows into the flame brush. The highly-deformed flame surface in the brush is spread out through the entire region between the reflected shock and the end-wall. The material is continuously burned by the flame oriented mostly parallel to the tube axis. Numerical Schlieren pictures generated from three-dimensional distributions of density show the apparent overall picture consisting of a reflected shock followed by a region of approximately constant-volume burning. This picture is consistent with, and gives an explanations of a strange reactive wave which is characterized by approximately half CJ velocity and significantly lower pressure, and which was observed in the experiments [1,2] before the system transitioned to a detonation. Details of the simulations are presented in [8].

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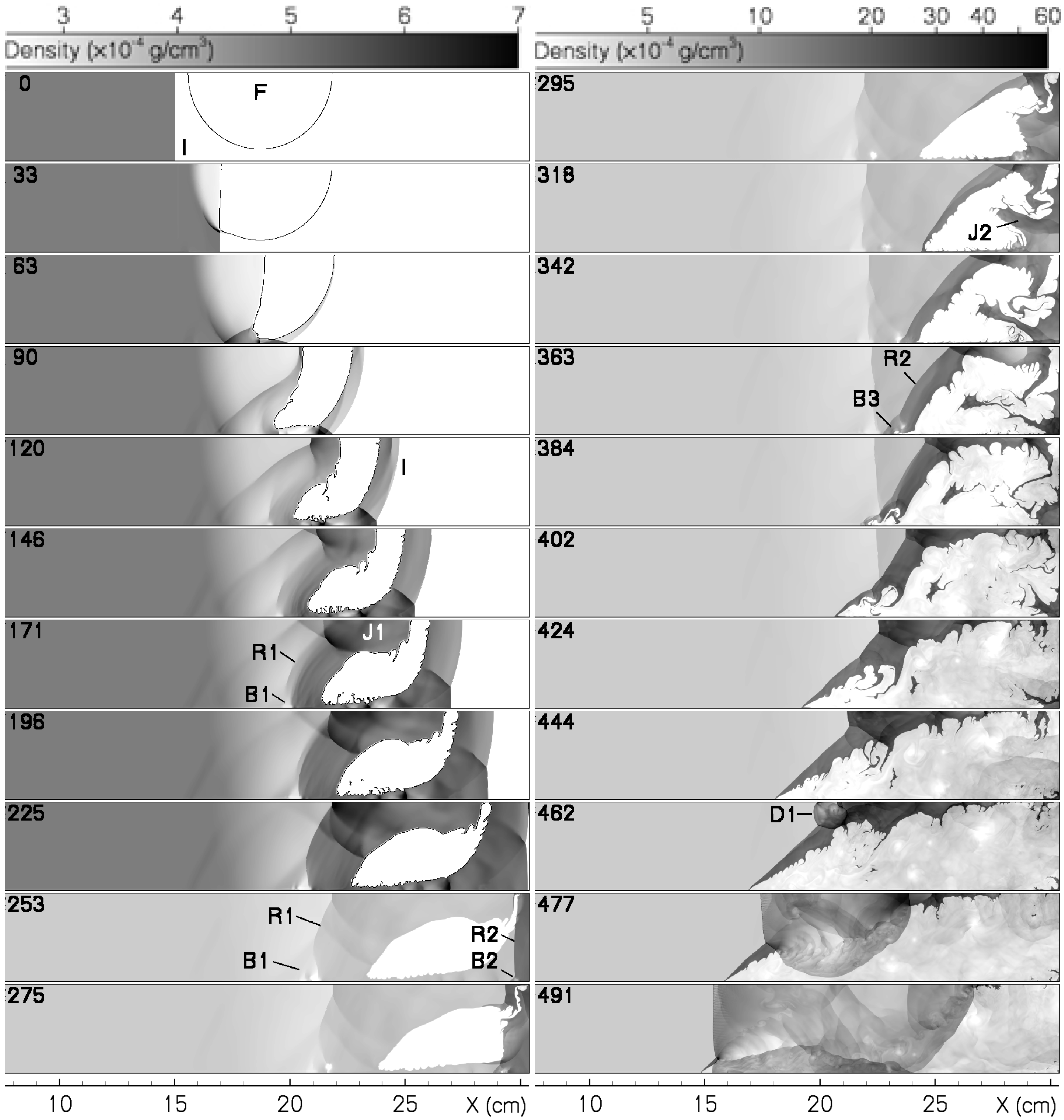

Figure 2. The overall picture of flow development in reflected-shock DDT simulation with $M_s = 1.9$. Time in microseconds is indicated on each frame. Left density scale is for times less than 253 microseconds. Various letters indicate flame (**F**), reflected shocks (**R**), bifurcated structures (**B**), Richtmyer-Meshkov funnels (**J**), and detonation (**D1**).

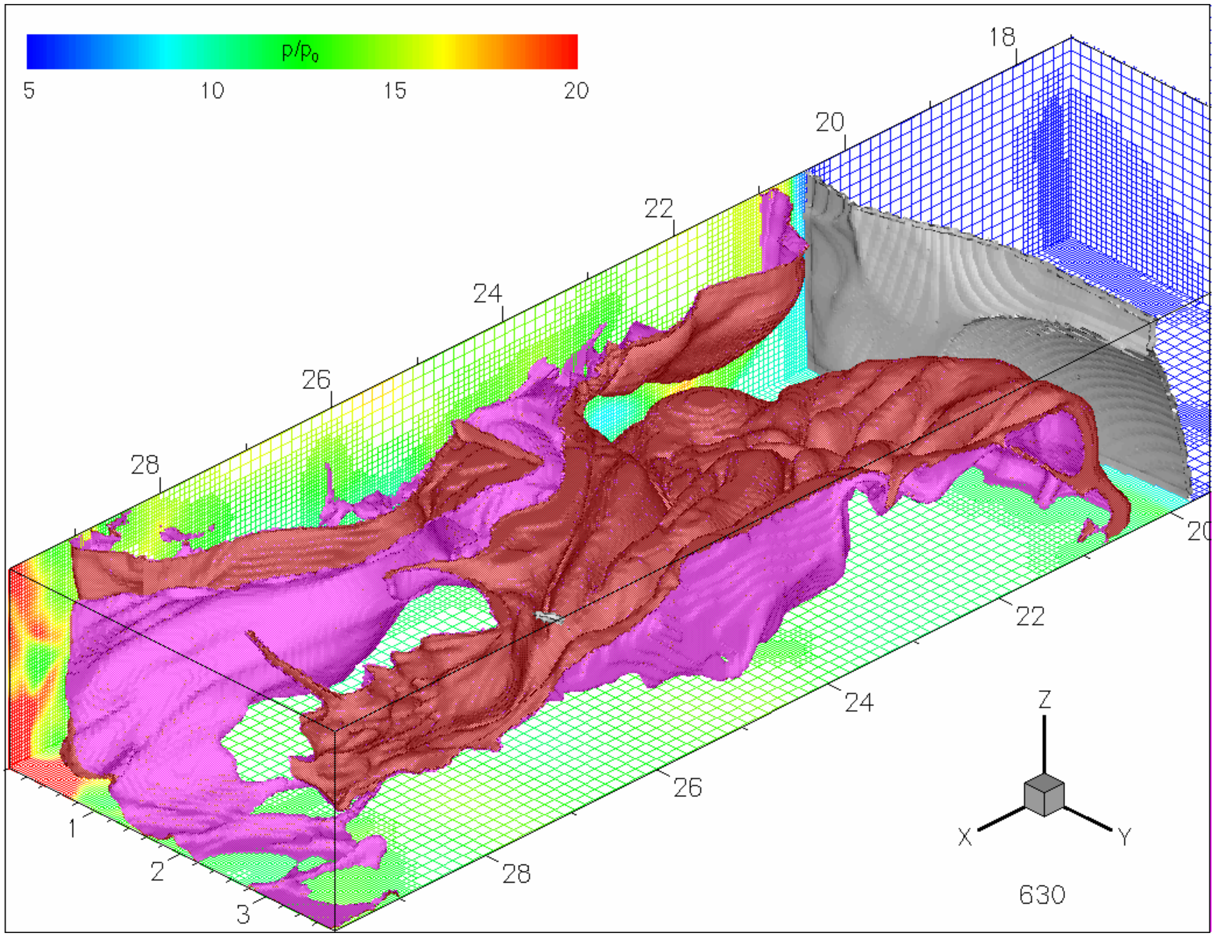

Figure 3. Flame surface (dark red side faces unburned mixture, purple side faces burned gas), main reflected shock (gray), and an adaptive mesh (mesh color shows the pressure) at 457 microseconds for a three-dimensional simulation with $M_s = 1.6$. Distances are in centimeters. Shown is a part of the computational domain adjacent to the end-wall which is located at X = 30.4 cm. Bottom X-Y and left X-Z sides of the domain are solid walls. Top X-Y and right X-Z sides are symmetry planes.

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