Soot motion in smoked foils

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1 Introduction

The soot track method, a simple and robust visualization tool, has been widely used to indicate detonation propagation, to measure the cell size and classify the regularity of cellular structure (Fickett and Davis [1]). Although it is obvious that the soot tracks are related to frontal shock waves, Pintgen and Shepherd [2] pointed out that triple-point trajectories measured by PLIF of the OH radical distribution near the soot foil are not exactly coincident with the soot tracks. Previous ideas about the mechanism of track formation has included pushing the soot with pressure gradients, "scrubbing" the soot off by vortices [3], and combustion of the soot in hot oxidizing atmospheres [4]. However, the precise physical mechanism that creates the soot tracks has never been clearly demonstrated. We proposed that the soot tracks depend largely on variations in the direction and magnitude of the shear stress created by the boundary layer over the soot foil. Our proposal is motivated by four key observations: 1) soot tracks can be formed in Mach reflection of a non-reactive shock [5], 2) pattern formation in oil flow visualization can be completely explained in terms of surface shear stress [6], 3) the process of Mach reflection in a non-reactive gas contains all the essential features of the shock configurations in detonation fronts, and 4) experiments [5] with soot patterns show streaks of soot indicating motion of the soot along the surface.

The goal of the present study is to explore explanations of track formation that are based on the classical fluid mechanics of near-wall flow in a viscous gas. We will perform a simulation of a 2-D detonation to detect the flow characteristics, and a simulation of a Mach reflection to estimate the shear stress and pressure distribution. Simple models of soot motions will be constructed and used to interpret the influences of shear stress, treating the soot layer as clumps of fine particles or an incompressible fluid.

2 Numerical setup

A flow field was computed for a detonation propagating is a stoichiometric $2H_2$+O_2+$2N_2$ mixture at the initial static pressure 20 kPa and static temperature 298.15 K. The C-J Mach number M_{CJ} and the half-reaction length $L_{1/2}$ are 4.92 and 452 μm, respectively. The 2-D Euler equations for a chemically reacting gas mixture are adopted as the governing equations. A 9-species, 19-reaction mechanism [7] is used for hydrogen-oxygen diluted by nitrogen combustion. Yee's non-MUSCL-type TVD upwind explicit scheme [8] is employed for the inviscid term in the equations. The computation is performed with a constant grid resolution of 50 grid points/$L_{1/2}$ along the x-axis. The channel width through which the detonation propagates is 3.6 mm (=8.0 $L_{1/2}$).
A simulation of a Mach reflection over a wedge is carried out at the similar condition of the frontal shock configuration as that observed in the detonation wave. The flow behind the shock wave is investigated by numerically simulating the 3-D compressible Navier-Stokes equations. Initial conditions are as follow; 298.15 K

static temperature, Mach 4.92 shock, an apex angle of the wedge θ_w = 33.1 degree, unit Reynolds number Re =1.8×10^7 m. As shown in Fig. 1, a stretched grid system is used and the number of grid points is 151×51×101 (5.3×0.7×3.6 mm). We adopt a shock-fixed coordinate system; the bottom *x-z* plane (a non-slip and isothermal boundary condition) corresponds to a soot foil and is moving at the same speed as the shock. The modeling of soot motion is carried out using two methods; the first is that the soot is treated as a continuum; the second is that the soot is regarded as an aggregate of solid particles.

Fluid model

Assuming that the soot can be approximated as an incompressible fluid, the soot thickness *h* can be expressed by the following conservation equation [6];

$$\frac{\partial h}{\partial t}+\frac{\partial(hu)}{\partial x}+\frac{\partial(hw)}{\partial z}=0\,,\quad u=\frac{\tau_{yx}h}{2\mu_s},\quad w=\frac{\tau_{yz}h}{2\mu_s} \qquad (1)$$

where u, w, τ_{yx}, τ_{yz} are the velocity components and the shear stresses arising from the gaseous boundary layer in *x* and *z* directions, respectively, and μ_s is viscosity of the soot layer. The governing equations (1) are discretized with MacCormack scheme [9] in a 2-D computational domain that has the same cross-sectional area of 3-D grid for the air (301×101 grid points) above the soot. Shear stresses of air drive soot motion, although soot-thickness distributions do not affect air flow; in other words, only one-way coupling is assumed.

Particle model

The discrete particle approach assumes that the soot layer is composed of spherical particles distributed in the *x-z* plane. The governing equations of soot particles are;

$$\frac{\partial \mathbf{I}_i}{\partial t}=\mathbf{F}_i\,,\ \mathbf{I}_i=\begin{bmatrix}x_i\\ z_i\\ u_i\\ w_i\end{bmatrix},\ \ \mathbf{F}_i=\begin{bmatrix}u_i\\ w_i\\ \left(f_x/m_p\right)_i\\ \left(f_z/m_p\right)_i\end{bmatrix} \qquad (2)$$

where $f_x=\pi\overline{\tau_{yx}}r_p^2$, $f_z=\pi\overline{\tau_{yz}}r_p^2$ are tractive forces for *x*, *z*-components, $m_p=4/3\pi\rho_s r_p^3$ and r_p are mass and radius of a soot particle, respectively, and ρ_s (=1200 kg/m^3) is soot density. The governing equations (2) are solved by the fourth-order Runge-Kutta method. Initially, 64 particles are arranged in each computational cell (300×100 cells).

3 Results and discussion

Preliminary simulation of 2-D Detonation

Frontal properties are examined to determine parameters for the Mach reflection simulation reproducing the shock configuration of the detonation wave. The key parameters for Mach reflection are the transverse wave strength, defined by the pressure jump across the reflected shock wave, and the entrance angle of triple-point track. Figure 2 indicates the instantaneous pressure contours of the detonation front. This frontal shock configuration is a double-Mach reflection (DMR). The transverse wave strength S (= p_3/p_1 - 1) is approximately 0.9, where p_1 and p_3 are the post-incident and the post-reflected shock pressures, respectively. Detonation history as presented by the maximum pressure contours is depicted in Fig. 3. The entrance angle of the triple-point track α is about 40 degrees, which corresponds to the desired transverse wave strength (S = 0.9) [1].

3-D Simulation of Mach reflection (Air, non-reactive gas)

Figure 4 illustrates the analogy between a detonation front and a Mach reflection over a wedge. The Mach reflection consists of the Mach stem and the incident shock wave as well as the incident detonation front. The summation of the track angle of a triple-point χ derived from the three-shock theory and an apex angle of the wedge θ_w equal the entrance angle α (= χ+θ_w). According to this relation, θ_w is determined to be 33.1 degree.

Figures 5 shows the instantaneous pressure distribution on the opposite side of the soot foil. At this location we observe the flow outside of the boundary layer induced by the shock wave. In the pressure distribution (Fig. 5), DMR can be seen, and the track angle of the triple point χ is about 9.4 degrees. The entrance angle α (= 42.1

degree) is in good agreement with that of the detonation case. The transverse wave strength equals to 0.8, which is close to the value of 0.9 in the detonation front.

Simulations of soot redistribution

Simulations of soot thickness are performed, using shear stress histories computed for the gas phase boundary layer. Figure 6 shows the soot thickness h normalized by the initial soot thickness h_0 with the fluid model in the form of gray-scale distribution. The shock front propagates from right to left. Soot is piled up around a triple-point track due to the kinks on the frontal and reflected shocks. While only one soot track is formed on the Mach stem side in SMR in our previous results [10], it is also formed on the incident shock side in DMR in the present study. In this model, parameters are initial soot thickness h_0 (= 1.7 mm) and soot viscosity. The soot viscosity is not well known and is approximated with the property of glycerin $\mu_{glycerin}$ (= 14.9×10^{-4} Pa s) at 298.15 K. As the initial soot thickness decreases with constant μ_s, soot track shows less contrast and finally disappears. The arbitrary viscosity coefficient can be chosen (e.g. μ_{air} = 18.2×10^{-6} Pa s) to obtain the same feature of soot tracks with the appropriate initial thickness (h_0 = 2.0 μm for air).

With the particle model, a result similar to the fluid model is obtained as shown in Fig. 7. Parameters in the particle model are initial soot thickness h_0 (= 20 μm) and particle radius r_p (= 0.27 nm). In this model, initial soot thickness is not important for contrast of the soot tracks, but the particle radius dominates the magnitude of soot thickness variations. Parameters are chosen by the same criterion as the fluid model and for this reason, the computational particle radius of 0.27 nm is much smaller than that of typical soot particle radius. Although drag force and skin friction do not affect the present results, consideration of additional forces, such as pressure gradients, may be necessary. Similar soot distributions are obtained by fluid and particle models by choosing appropriate parameters.

4 Summary

Soot track formation was numerically investigated, assuming that the soot tracks are due to variations in the direction and magnitude of the shear stress created by the flow in the gas boundary layer over the soot foil. A two-dimensional $2H_2+O_2+2N_2$ detonation was simulated to examine frontal properties and determine the parameters for Mach reflection simulation to reproduce the same shock configuration as detonation. In non-reactive air, double Mach reflection appeared by using the determined parameters, and shear stress vectors suddenly changed their directions across the triple point and a reflected shock. Using the computed gaseous shear stress, similar soot distributions are obtained by fluid and particle models by choosing appropriate parameters. Soot is piled up around a triple-point track due to kinks (triple points) on the frontal and the reflected shocks. While a soot track is only formed on the Mach stem side in single Mach reflection, it is also formed on the incident shock side in double Mach reflection.

References

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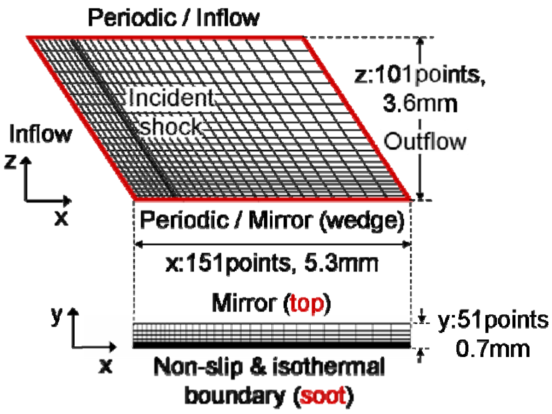

Fig. 1 Computational domain and boundary conditions.

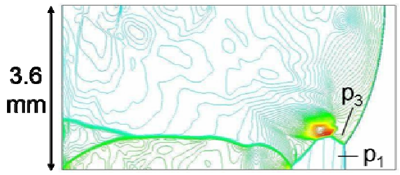

Fig. 2 Instantaneous pressure contours (post-shock pressures; p_1, incident shock; p_3, reflected shock).

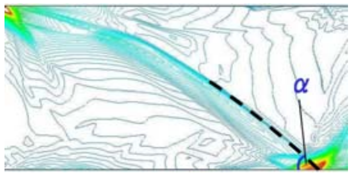

Fig. 3 Maximum pressure history (α, the entrance angle of the triple point track).

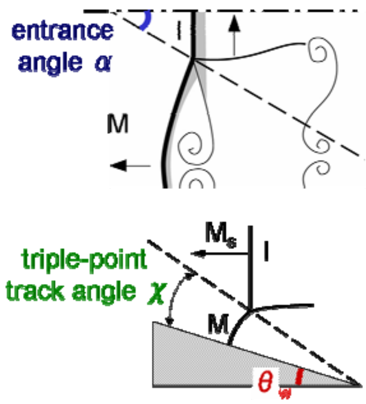

Fig. 4 Analogy between the detonation and the Mach reflection over a wedge.

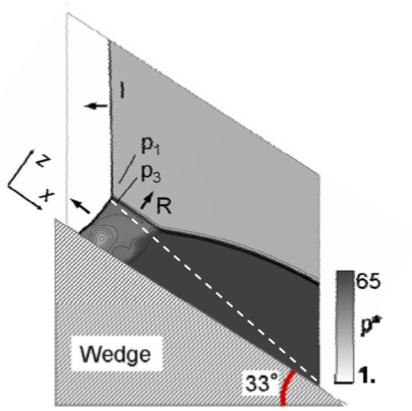

Fig. 5 Instantaneous pressure distribution on the opposite side of the soot foil.

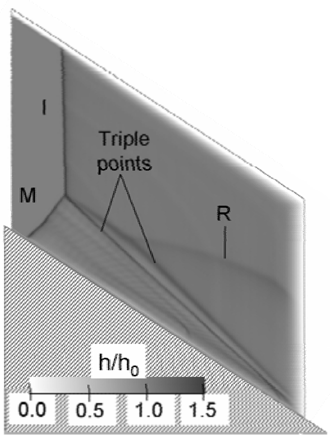

Fig. 6 Soot thickness distribution by fluid model.

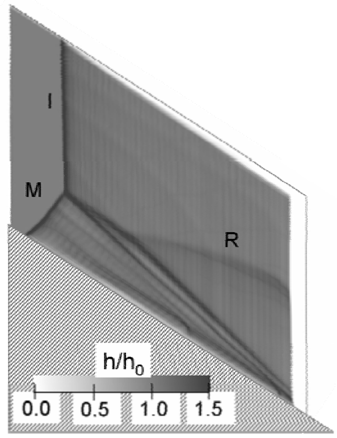

Fig. 7 Soot thickness distribution by particle model.