One-dimensional Evolution of Fast Flames

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1 Introduction

Since laminar flames are usually slow compared to the sound speed, the laminar flame theory [1] largely ignores effects of compressibility. For example, the steady-state solution [1,2] of transport and energy-release equations provides the flame velocity and profile assuming a constant pressure. If this profile is used as an initial condition for a time-dependent solution of Navier-Stokes equations, it may remain the same or change significantly depending on the flame velocity. Here we consider the evolution of fast flames that propagate at more than 20% of the speed of sound. Laminar flames with such speeds are rather exotic and still relatively unexplored, though they may occur in real systems. Understanding their evolution may also help to understand the behavior of fast turbulent flames.

2 Numerical Model

The numerical model is based on reactive Navier-Stokes equations coupled with the ideal-gas equation of state

$$e = P/(\rho(\gamma - 1)), \quad T = (m/R) P/\rho \tag{1}$$

and a one-step Arrhenuis kinetics of energy release

$$w_q = q \left(\frac{dY}{dt} \right) = -q A \rho Y \exp(-E_a/RT), \tag{2}$$

where w_q is the energy release rate, q is the chemical energy release per unit mass, Y is the unburned mass fraction, A is the pre-exponential factor, and E_a is the activation energy. Transport properties are represented by thermal conduction K and diffusion D coefficients that depend on temperature as

$$K/\rho C_p = k_0 T^n, \quad D = D_0 T^n/\rho \tag{3}$$

where k_0 and D_0 are constants, n = 0.7, and $Cp = \gamma R/M(\gamma - 1)$ is the specific heat. To simplify the analysis, we assume the unity Lewis number, that is $k_0 = D_0$, and neglect viscosity, which has little effect

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on the results. The equations are solved using the explicit, second-order, Godunov-type numerical scheme incorporating a Riemann solver, and the FTT-based structured adaptive mesh [3].

To generate initial conditions for time-dependent simulations, and compute key physical scales, we use steady-state models for laminar flames and ZND detonations described in [2]. The flame thickness x_l is defined as $x_l = (T_b - T_0)/(dT/dx)_{max}$, where $T_b = T_0 + q/C_p$ is the post-flame temperature, and $(dT/dx)_{max}$ is the maximum temperature gradient in the flame profile. The detonation thickness x_d is defined as the distance between the shock and the half-reaction Y = 0.5 plane.

Numerical resolution used in time-dependent simulations was sufficient to resolve all relevant length scales, such as x_l and x_d , with multiple computational cells. Resolution tests were performed to make sure that all results discussed in this work are independent of the computational cell size.

Parameters of the reactive system are based on the set of parameters defined in [2] for a stoichiometric hydrogen-air mixture. The model system that we consider here, however, is far from hydrogen-air since we vary A and k_0 by several orders of magnitude. All parameters of the equation of state, q, and E_a are kept constant.

3 Fast Flames

The flame velocity S_l in the steady-state model depends on the rate of energy release, which is proportional to A, and the thermal conductivity, which is proportional to k_0 . It can be shown that S_l is proportional to $\sqrt{k_0}$ and \sqrt{A} , which means that $S_l = const$ for $Ak_0 = const$. On the other hand, the flame thickness x_l is proportional to $\sqrt{k_0}$ and $\sqrt{1}/A$, which means that flames may have the same speed but different thicknesses. In the framework of the current numerical model, the flame thickness only plays a role of a length scale. Solutions obtained for different x_l , but the same S_l are self-similar. Because of that, the flame evolution in a dimensionless space scaled by x_l is controlled by only one independent parameter S_l (or Ak_0).

We therefore consider the evolution of one-dimensional flames for a series of Ak_0 that correspond to different S_l scaled by the sound speed c_0 in the cold unburned material. For the original parameter set corresponding to hydrogen-air mixture, $S_l/c_0 = 0.008$ and the results of time-dependent Navier-Stokes simulations reproduce the steady-state solution with the accuracy $\sim 0.1\%$ with respect to the flame speed [2].

When both A and k_0 are increased by a factor of 27, S_l/c_0 increases to 0.215. The flame evolution computed for this case is shown in Fig. 1. The time-dependent solution produces a weak shock ahead of the flame that modifies background conditions. The propagating flame readjusts its velocity and structure to these new conditions. This new flame structure can be considered as approximately steady-state. Though the distance between the flame and the shock gradually increases, as does the residence time for the material in the shock-compressed layer, the temperature behind the weak shock is too low to cause any substantial chemical reaction on reasonable time scales.

Further slight increase of S_l/c_0 to 0.264 changes the flame evolution drastically. The results of timedependent simulations in Fig. 2 show that a strong pressure pulse grows within the flame and significantly alters its structure. The pressure pulse and the flame quickly couple to each other producing a thick reactive shock that propagates at a constant velocity above D_{CJ} . The structure of this reactive wave is well resolved with about 30 computational cells. A detailed analysis shows that this wave is a self-supporting weak detonation, and it is the final steady-state for fast flames evolving in our model system. Weak detonations is a well-know theoretical concept that follows from the analysis of detonations in P-V diagram [1], but they usually lack a self-supporting mechanism of propagation in real systems. They are often considered as artificial combustion waves that can be created if an external ignition source (for example, a laser beam) ignites the material with a prescribed velocity above D_{CJ} . Know natural phenomena that can be considered as weak detonations are condensation shocks [1] and transient spontaneous reaction waves that propagate through a reactivity gradient [4,5].

Weak detonations as solutions of Navier-Stokes equations have been analyzed in detail in [6], and also observed in numerical simulations [7] when the reaction rate for ozone decomposition was increased by a factor of 5. A strong shock propagating at the velocity equal to D_{CJ} was used as the initial condition in these simulations. Authors noted that the observed wave is supersonic both from the front and back, but no further analysis has been performed in [7].

To understand the conditions when such self-supporting weak detonations may form, we need to consider two relevant length scales: the thickness of the shock x_s and the thickness of ZND detonation x_d . Usually $x_d \gg x_s$, the reaction starts behind the shock, and a regular ZND detonation forms. The reaction can occur inside the shock when x_s become comparable or larger than x_d . Since the Arrhenius reaction rate is mostly affected by the temperature, we will consider the thermal thickness of the shock $x_s = (T_{ZND} - T_0)/(dT/dx)_{max}$, where T_{ZND} is the temperature behind ZND shock, and $(dT/dx)_{max}$ is the maximum temperature gradient inside the shock. In our model, x_s is proportional to k_0 , and x_d is proportional to 1/A. This means that there are multiple combinations of k_0 and A that give $x_s/x_d = 1$, but all of them correspond to the same $Ak_0 = const$. As we explained above, this also corresponds to a particular flame velocity S_l .

The flame velocity itself is not relevant for the analysis of the structure of weak detonations, but can be used instead of Ak_0 combination to compare domains of existence of weak detonations and accelerating flames that lead to detonations. Calculations show that for our model parameters, $x_s/x_d = 1$ corresponds to $S_l/c_0 = 0.22$. As we have shown, this flame speed is very close to the boundary between accelerating and non-accelerating flames. Larger S_l correspond to larger Ak_0 , and therefore to $x_s/x_d > 1$. Thus all flames in our model system that are fast enough to evolve into detonations should evolve into weak detonations, and this is what we observe in our simulations. For any model parameters, including those corresponding to slower flames, detonations can be initiated by strong shocks. Detonation regimes observed are independent of the initiation mode.

The detonation regimes computed for different x_s/x_d are shown on the P-V diagram in Fig. 3. Here black lines show the unreactive Hugoniot and Raleigh line for the CJ detonation. Blue dots correspond to weak detonations that propagate with velocities higher than D_{CJ} . Green line is still a weak detonation that completely burns the material inside the shock, but propagates with velocity close to D_{CJ} . Red dots correspond to intermediate detonation regimes for which the material partially burns inside the shock, and partially behind the shock along the Raleigh line. The detonation velocity for these regimes is equal to D_{CJ} .

Scattered red dots connected by dotted lines below the Raleigh line are inside the unresolved part of the shock that appears because of zero viscosity. They approximately correspond to Hugoniots of partially reacted material that start on the Raleigh line below CJ point (dotted line begins) and end on the Raleigh line above CJ point (dotted line ends). After the shock compression along these Hugoniots, the material expands as it continues to burn along the Raleigh line.

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Reaction-zone profiles computed for weak and intermediate detonation regimes are shown in Fig. 4. According to the Mach number profiles, the flow behind a weak detonation is always supersonic. This means that the flow cannot be affected by a rarefaction originating from a boundary behind, and this is why the pressure behind the reaction zone remains constant. For intermediate detonation regimes, the part of the reaction zone behind the shock is subsonic, but the flow becomes sonic as the reaction ends. This is consistent with P-V diagram in Fig. 3 which shows that for these regimes the reaction ends at CJ point.

Finally, we note that one-dimensional ZND detonations in the model system considered here are unstable. The steady-state ZND profile shown in Fig. 4 for $x_s/x_d = 0$ cannot be obtained in time-dependent simulations and was computed using steady-state equations. Weak and intermediate detonation regimes computed here are stable for $x_s/x_d > 0.1$, shows a slight instability for $x_s/x_d = 0.093$, and are severely unstable for $x_s/x_d < 0.05$. This is consistent with the analysis [8,9] which concludes that weak detonations are stable.

5 Conclusions

We consider the evolution of very fast laminar flames in a model system. One-dimensional time-dependent computations based on Navier-Stokes equations show that these flames tend to accelerate when the flame velocity computed from a steady-state model is above 22% of the speed of sound. The flame evolution leads to a new steady-sate which is a detonation. When model parameters allow the shock to become thicker than the reaction zone of ZND detonation, we observe self-supporting weak detonations that burn the material inside the shock and propagate with velocities above D_{CJ} .

For the model system considered here, the range of parameters for which flames accelerate coincides with the range of parameters for which weak detonations exist. In general case, however, these two phenomena are not related to each other. For example, a turbulent flame in a reactive gas mixture may become fast enough to produce a detonation, but this will be a regular ZND detonation since the shock will remain thin compared to the reaction zone. Weak detonations can be expected when a large preheat zone can form ahead of a shock, for example due to a radiation heat transfer.

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Figure 1: Time sequence of pressure and burned mass fraction profiles showing the evolution of a laminar flame for $S_l/c_0 = 0.215$. The beginning (a) and the continuation (b) of the evolution are shown on different scales.



Figure 2: Time sequence of pressure and burned mass fraction profiles showing the evolution of a laminar flame for $S_l/c_0 = 0.264$. The beginning (a) and the continuation (b) of the evolution are shown on different scales.



Figure 3: P-V diagram for steady-state detonation regimes computed for different x_s/x_d (values shown). Blue and green dots correspond to weak detonations. Red dots correspond to intermediate detonation regimes.



Figure 4: Steady-state reaction-zone profiles for weak (a) and intermediate (b) detonation regimes. Values of x_s/x_d are shown at the top. ZND profile corresponds to $x_s/x_d = 0$. Flow Mach number M is computed in the frame of reference of the shock.