DEFLAGRATIONS, HOT SPOTS, AND THE TRANSITION TO DETONATION

Elaine S. Oran* and Alexei M. Khokhlov*
Laboratory for Computational Physics and Fluid Dynamics
Naval Research Laboratory, Washington DC, USA

Introduction and Background

Deflagration-to-detonation transition (DDT) is an extremely complex physical process involving deflagrations, shocks and shock reflections, boundary layers, and all of their interactions with each other. Exactly how DDT occurs is not clear from experiments, and seems to vary from event to event. One useful way of studying DDT has been in shock-tube experiments. A flame, ignited by a spark at one end of a tube, propagates along the tube, develops into a turbulent flame brush, and may eventually transition to a detonation [1]. In another approach, a turbulent flame brush was created through repeated shock-flame interactions in reflected-shock-tube experiments [2,3]. In both situations, the location of the explosion that leads to DDT varied from case to case, depending on initial and material conditions.

Hot spots (also called reactive centers or exothermic centers) are important elements of detonation initiation. The gradient mechanism of the initiation of a detonation [4] (also called SWACER [5]) describes how a hot spot may evolve into a detonation. The principal feature of this mechanism is the presence of the gradient of induction time that leads to a spontaneous reaction wave which, under the appropriate conditions, may transition to a detonation. There is now substantial experimental and theoretical evidence that a detonation can be triggered by such a gradient [6–10].

Our previous work described how turbulence can at least partially extinguish a flame and create gradients that allow DDT in unconfined conditions [9]. Now we have completed a series of computations that investigate how DDT may suddenly occur in a confined acetylene-air system containing a turbulent flame [11–13]. In this presentation, we bring together these and newer results for etheylene-air and use them to discuss mechanisms of DDT. In particular, we discuss the role of dimensionality, turbulence intensity, boundary layers, and the dynamic behavior of hot spots in creating conditions in which DDT can occur.

Problem Description

The simulations modeled a flame ignited in a closed tube and then hit with an incident and reflected shocks. Repeated shock-flame interactions resulted in a highly turbulent flame brush. The computations solved the multidimensional, time-dependent, reactive Navier-Stokes equations including the effects of compressible fluid convection, chemical reactions with subsequent energy release, molecular diffusion, thermal conduction, and viscosity [11]. The materials used in both the experiments [3,14,15] and computations were low-pressure mixtures of either ethylene or acetylene with air (100 Torr, 298 K). The location of the flame in the tube and the strength of the incident shock, M_s, were varied. A simplified single-step Arrhenius chemistry model was developed that gives the correct one-dimensional flame and detonation properties over a range of temperatures and pressures typical of the experiments.

To compute DDT from the basic principles of reactive flow, it is necessary to resolve the largest and smallest relevant scales in the system, where and when they are important. This means resolving a range of scales from the length of the tube (32 cm) to the laminar flame thickness (tenths of millimeters). For this reason, the model was solved on a dynamically adapting mesh called the Fully Threaded Tree (or FTT) [16]. The adaptive mesh also ensured that shocks, flames, and incipient hot spots were well resolved.

Summary of Simulation Results

The acetylene-air experiments involved a vertical row of merging flames that were hit by incident shocks [5,14]. The simulations modeled a portion of the problem in the center of the tube, using symmetry boundary conditions [12,13]. Incident shock strengths were in the range $M_s = 1.4 - 1.63$. These computations showed the following general features:

1. The interactions of an incident shock with the initially laminar flame lead to the formation of secondary shocks and rarefactions that continued to distort the flame surface, eventually creating a turbulent flame brush.

* Mailing Address: Code 6404, Naval Research Laboratory, Washington DC 20375, USA
E-mail — E.S. Oran: oran@lcp.nrl.navy.mil; A.M. Khokhlov: ajk@lcp.nrl.navy.mil

2. The turbulence in the flame brush was continuously driven by shock-flame interactions which populated the turbulence scales considerably more than the Kolmogorov cascade.
3. Pressure fluctuations, generated by shock-flame interactions in the flame brush, were the seeds for hot spots in unreacted material.
4. There were gradients of the induction time inside the hot spots. When the conditions in the gradient regions were appropriate, supersonic spontaneous waves resulted, and these transitioned to a detonation. In other cases, the hot spots resulted in a decoupled system of a shock wave and a flame left burning behind it.
5. Detonation ignition occurred in unreacted material in which the critical size of the gradient required for DDT was significantly reduced due to shock heating and compression.
6. As M_s was increased, intensity of the turbulent flame brush increased and the location of DDT event shifted from unreacted material outside the flame brush to unreacted material within the region of the flame brush.
7. The turbulence itself was not strong enough to extinguish the flame to any appreciable degree, so that the flame surface appeared intact. This might change as the chemical model is made more realistic and complex.

The ethylene-air computations involved a single spherical flame hit by incident shocks in the range $M_s = 1.4 - 1.8$. The walls of the tube were assumed to be adiabatic. These calculations showed all of the same effects noted above, plus others due to the formation of boundary layers on the walls. In particular, these showed:

8. Comparisons of two- and three-dimensional computations show that ignition occurs sooner in three dimensions, consistent with the differences noted in the two- and three-dimensional shock-flame interaction studies [11]. However, the basic mechanism of ignition, a hot spot developing in a gradient, is the same in all of the computations to date.
9. As in the acetylene computations, there is a noted lack of distributed flames. The distributed flames seen in the computations do not seem to contribute to the DDT event. In the case of ethylene, however, the absense of distributed flames is even more likely to be an effect of the simplifed chemical reaction model.
10. Boundary layers were formed on the walls as shock and flame fronts moved through the system. The material at the boundary was slowed and heated, and created regions in which flames developed. These flames propagated in to the system from the boundary layer. When yet another shock hit these expanding flames, the interaction was a standard shock-flame interaction that created a turbulent flame with wrinkling generated on the scale of a few laminar flame thicknesses. This is a possible exlanation for the observations of coupled shock-flame complexes observed in experiments [15].

Discussion

There are two different conceptual approaches to understanding the origin of DDT. In one, DDT results from regions which have gradients in induction time [4–10]. These gradients then allow spontaneous waves to arise, and these transition to a detonation. In the second approach, hot spots are caused by fluctuations in the material and, given the right conditions, a detonation occurs by an explosion of a hot spot [18]. For the computations we have shown, these two theories are not rivals, but consistent with each other. What we have shown is that the hot spots do arise from fluctuations whose level increases as the turbulent flame become becomes more intense. Then the actual physical mechanism by which a hot spot explodes and creates a detonation is by generating a spontaneous wave that arises due to gradient of induction time.

We believe that the basic principles needed to describe the two different situations, unconfined and confined, may be used to describe intermediate situations. For example, in jet initiation of DDT [19–21], a jet of turbulent of reacted hot material is injected into cold, premixed material. For DDT to occur, the turbulence should be of the right scale (strength and size) to mix enough hot and cold material, and so create conditions of a distributed flame that would lead to DDT. Weak shocks, generated by unsuccessful hot-spot explosions, could help prepare the medium for DDT. This description, based partly on speculation and partly on extrapolation of what we know, should be tested with simulations.

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