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# **Flame Acceleration and Transition to Detonation in High-Speed Turbulent Combustion**

Final report for ONR Contract number N000141410177  
for the time period December 31, 2013 – December 31, 2016

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## **Abstract**

The objective of this project is to address the grand-challenge question in combustion dynamics: How and under what circumstances does a flame propagating in a smooth channel accelerate to the point where there is a transition to detonation (DDT)? We are also asking: What are the specific physical mechanisms controlling this process? Work has progressed on five fronts: (1) Clarifying the route to DDT as the channel geometries change from large to small flow blockages; (2) Finding the mechanism of DDT in small, smooth channels; (3) Finding adequate and simplified models for chemical and diffusion processes for use in complex reactive-fluid-dynamics simulations of hydrocarbon combustion; (4) Determining the effects of surface roughness on DDT; and (5) Determining the effects of acoustic-flame-boundary interactions in closed channels containing fuel-air mixtures.

# Flame Acceleration and Transition to Detonation in High-Speed Turbulent Combustion

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# Flame Acceleration and Transition to Detonation in High-Speed Turbulent Combustion

## 1. Introduction to the Challenge Problem

The importance of high-speed turbulent combustion of gas mixtures and sprays is difficult to overestimate, as it is the main process in all internal-combustion engines used for propulsion and energy generation. These include piston engines, gas turbines, various types of jet engines, and some rocket engines. On the other hand, preventing high-speed combustion is critical for the safety of any human activities that involve handling of potentially explosive gases or volatile liquids. Thus, the development of more fuel-efficient, safer, and more affordable technologies and systems depends on a good understanding of all mechanisms involved in high-speed combustion and the ability to use this knowledge in numerical simulations.

High-speed turbulent combustion can involve two distinct types of combustion waves, deflagrations and detonations. Deflagrations are relatively slow (subsonic), and currently used in all commercial internal combustion engines. In some configurations, deflagrations (flames) can accelerate and produce detonations that propagate with supersonic velocities, and these can be extremely destructive. Currently, detonations are used in experimental pulse-detonations engines (PDE) and rotating-detonation engines (RDE) that potentially can be more efficient than deflagration-based turbines.

The process of flame acceleration and deflagration-to-detonation transition (DDT) depends on the mixture composition and the geometry of the confinement. Although there have been considerable advances in the last 10–15 years, the physical complexity means that it is still far from understood or controllable [1–5]. This process includes multiple complex phenomena such as turbulence generation, flame-turbulence interactions, generation and amplification of shocks, and initiation of a detonation. The lack of clear understanding of these phenomena is related to their complex multistage and multiscale nature. Because of that, detailed experimental diagnostics that might reveal key mechanisms are difficult, expensive, and often incomplete or unavailable. Detailed numerical simulations that reproduce available experimental data can fill gaps in experimental diagnostics and help to understand essential mechanisms. Such simulations, however, also have to deal with multiple length scales and often push the limits of existing computing capabilities.

Now we have combined state-of-the art numerical simulations and available experimental data to help decipher the detailed mechanisms of flame acceleration and DDT in gas mixtures. The overall goal of the proposed work is to answer one of the Grand-Challenge problems of turbulent reactive flows, *What is the mechanism of transition to detonation in a perfectly smooth channel?* The approach to the problem was to develop the multiphysics, multiscale, multidimensional, unsteady, fully compressible numerical models needed to describe the phenomenon, and then to use these models to simulate a series of flows that will give us insight into this transition process.

The currently completed study has provided fundamental knowledge and modeling capabilities for high-speed combustion processes that can be used to accelerate the development of more efficient, and more affordable propulsion technologies and systems. This work is equally important for the safety of storage, transportation, and use of fuels, including the safe operation of ships, vehicles, and devices powered by hydrogen fuel cells, which is also closely related to the affordability of naval systems operations.

## 2. Background on Previous Research

Over the past two decades, numerical simulations have been used in conjunction with carefully designed experiments to learn a great deal about the physical mechanisms controlling flame acceleration and DDT in gaseous systems. Our research group, originally at the The Laboratory for Computational Physics and Fluid Dynamics at the Naval Research Laboratory and now joined with the University of Maryland, has played a central role in these developments. Our general approach has been to perform simulations using numerical methods and adaptive gridding techniques that allow us to resolve all physically relevant length and time scales. Details of this approach and its early applications are summarized in [6]. Since then, in 1999, members of our group have performed the first numerical simulation of DDT resulting from shock-flame interactions [7], in 2007, the first numerical simulation of DDT in obstructed channels [8], and, in 2011, the first numerical simulation of DDT resulting from flame-turbulence interactions [9]. Each of these pioneering studies resulted in a significant progress in our understanding of the combustion phenomena considered in this proposal. Here we briefly summarize our DDT results that are most relevant to the proposed project.

## *2.1 Shock-Flame Interactions and DDT*

The overriding objective of the first computations of shock-flame interactions with resolved flame surfaces was to determine if we could compute DDT from first principles [7,10,11]. More specifically, we wanted to determine if we could resolve a large enough range of the temporal and spatial scales to see the transition to a detonation. At the minimum, this would require resolving spatial scales from the laminar flame thickness to the size of the system. The approach we used combined numerical simulations with comparisons to laboratory experiments on shock-flame interactions in an attempt to find mechanisms responsible for unexplained observations. These simulations showed an important role of Richtmyer-Meshkov instabilities in increasing the surface area of the flame and thus the energy-release rate, shock amplification, formation of hot spots, and finally detonation initiation. Details of these simulations are shown in Figure 1 (left side) and described in the figure caption.

One important conclusion of this work was that detonations develop from hot spots that appear in shock-compressed material when shocks become strong enough. High-resolution computations showed that these hot spots are, in fact, small regions with temperature gradients that support the creation and propagation of spontaneous reaction waves. For a certain range of temperature gradients and hot-spot sizes, these waves evolve into detonations in accordance with Zeldovich's reactivity gradient mechanism [1,11].

The next series of studies of shock-flame interactions [12–14] analyzed the role of boundary layers and wakes on flame acceleration and DDT. We discovered reactive bifurcated structures that can develop when shocks interact with flames and boundary layers or other velocity gradients. The flow pattern associated with these structures causes flames to spread at shock velocities and leads to shock acceleration. When shocks become strong enough, hot spots appear in shock-compressed material, and detonations develop through the gradient mechanism. This process is shown in Figure 1 (right side) and explained in more detail in figure caption.

## *2.2 Flame Acceleration and DDT in Channels with Obstacles*

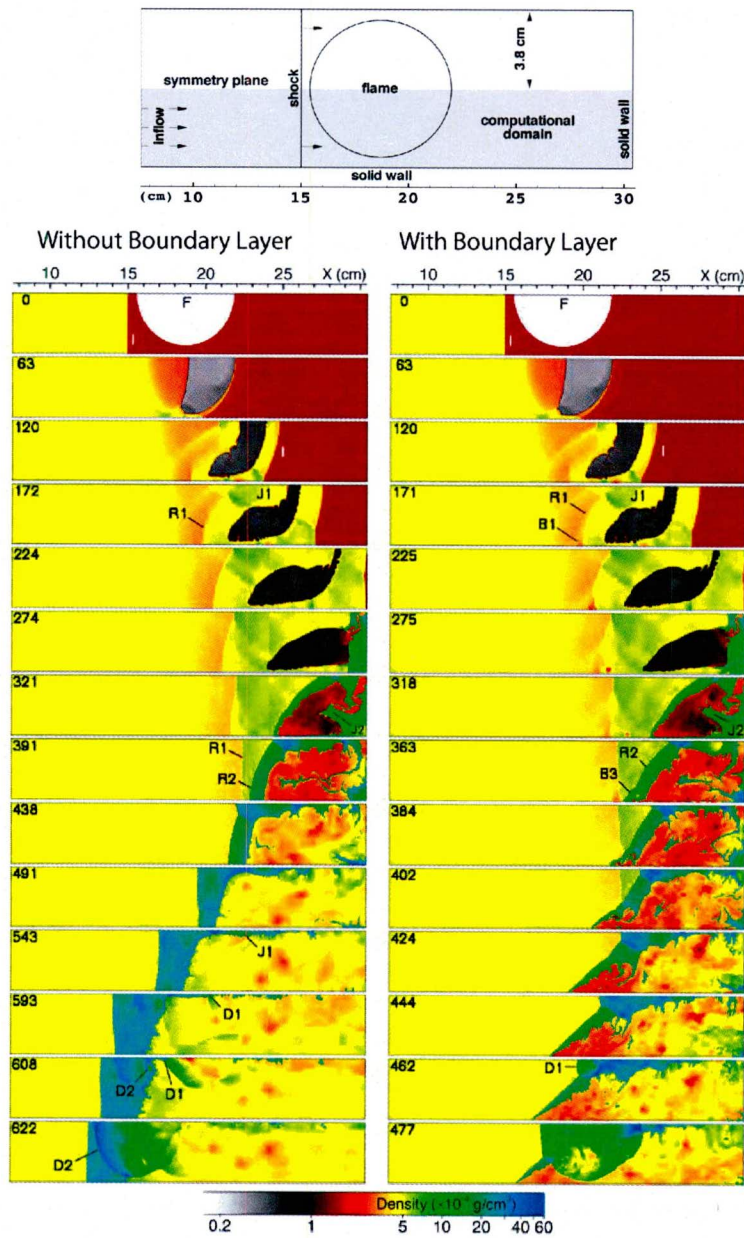
The DDT phenomena described above resulted from interactions of externally imposed strong shocks with a pre-existing flame. This setup creates a well-controlled environment

for DDT studies, but it also simplifies the problem. In practical systems, high-speed flames and shocks naturally appear as a result of the evolution of a slow laminar flame ignited by a spark. To include these initial stages of flame acceleration and shock generation, we considered flame acceleration and DDT in obstructed channels.

Channels with obstructions along the walls are prototype geometries used to represent various industrial settings. Our work on flame acceleration and DDT for these configurations was started to assess the safety of two specific industrial environments: hydrogen fuel storage stations and underground coal mines. The simulations in mixtures of hydrogen and air [1,3,8,15] and methane and air [16] have shown that basic mechanisms for the flame and flow acceleration observed in channels with obstacles involve thermal expansion of combustion products, shock-flame and flame-vortex interactions, and Rayleigh-Taylor, Richtmyer-Meshkov, and Kelvin-Helmholtz instabilities. The accelerating flow generates strong shocks that reflect from obstacles and eventually create hot spots that produce detonations through the gradient mechanism. Examples of simulation results with explanations are shown in Figure 2.

The simulations reproduced key experimental observations including three regimes of supersonic flame propagation in obstructed channels: choking flames, quasi-detonations, and detonations. Initial studies of stochasticity (that is, the stochastic properties of this turbulent reacting flow) have shown that there is considerable uncertainty in the computed time and location for detonation initiation. This is, in fact, consistent with the stochastic behavior observed in experiments.

We also studied the influence of geometrical parameters on flame acceleration and DDT. This work was expanded to unconfined arrays of obstacles that are more representative of industrial environments. The results have shown that the mechanisms of flame acceleration and DDT in these environments are similar to those in obstructed channels.



**Figure 1.** Effect of boundary layer on shock-flame interactions and DDT. This figure is taken from one of the first computations of the effects of boundary layers on shock-flame interactions and DDT [12] showing DDT arising from a gradient of reactivity in the flow [7]. The schematic on the top shows the conditions simulated, which were modeled on experiments performed at the University of Wales Aberystwyth. The sequence of density fields showing shock-flame interactions and DDT in a stoichiometric ethylene-air mixture at  $P_0 = 1.44 \times 10^3$  Pa for initial and boundary conditions shown on top.

*(Caption continued on next page.)*



**Figure 1.** (Continued).

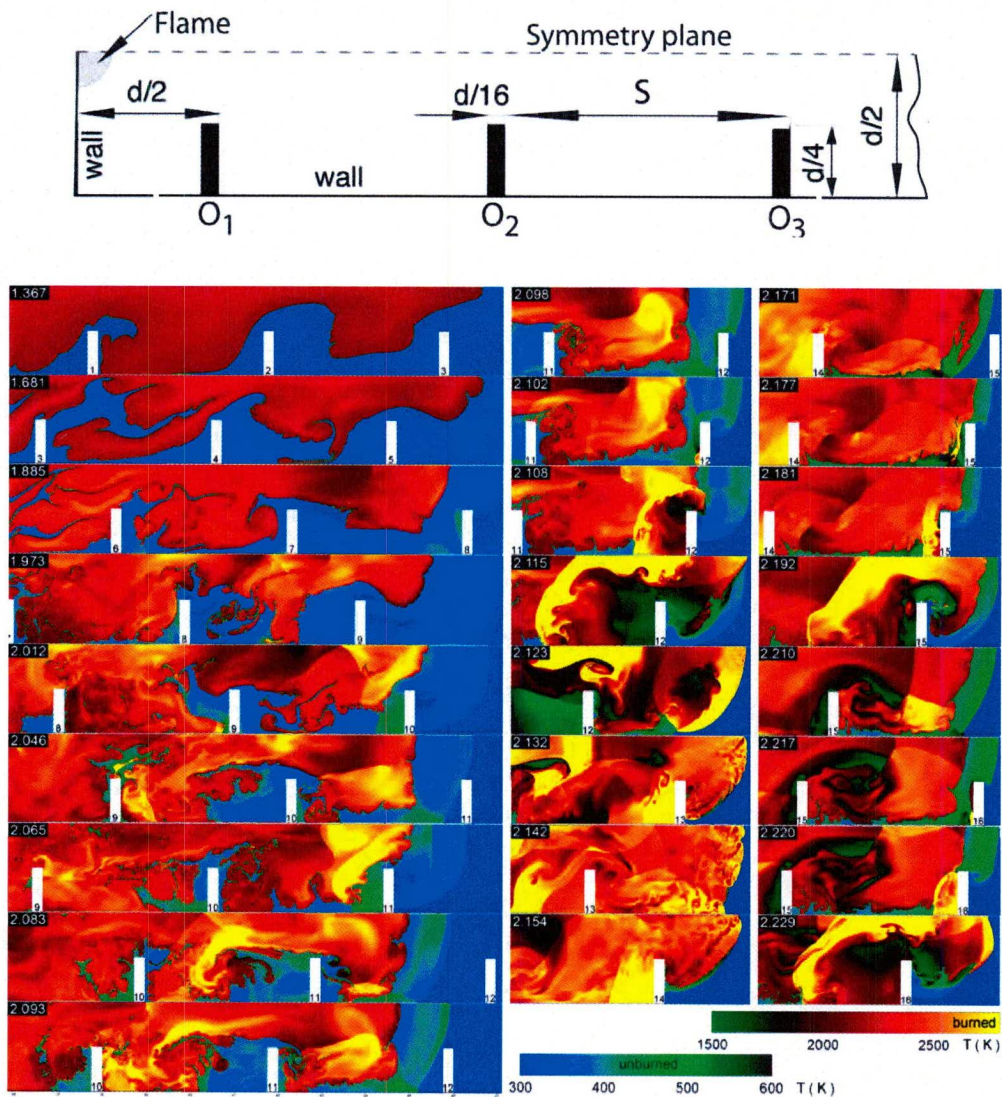
Two cases, with and without boundary layer were computed. Incident shock Mach number  $M_s = 1.9$ . Time ( $\mu s$ ) is given on the left side of each frame. The letters indicate the incident shock I, the flame F, reflected shocks R1 and R2, funnels of unreacted material J1 and J2, detonations D1 and D2, and bifurcated structures B1, B2 (not shown) and B3.

The sequence on the left is taken from a simulation with free-slip boundaries that suppressed the formation of a boundary layer. The first frame at  $0 \mu s$  shows the initial conditions, a planar incident shock I moving from the left to the right, and the flame F. The sequence of frames, with time increasing from top to bottom, shows the incident shock I moving through and distorting the flame, reflecting from the back wall, and then the reflected shock R2 passing through and further distorting the flame. Hot spots form in unreacted material, and eventually two of the hot spots undergo transitions to detonations at  $593 \mu s$  and  $608 \mu s$ .

The sequence on the right shows the development of the flow for the same mixture and value of  $M_s$ , but now for the case with a no-slip wall that allows a boundary layer to form. The boundary layer behind the incident shock is about  $0.1 \text{ cm}$  thick and is not visible in these frames. From the beginning of the simulation to about  $225 \mu s$ , the flow development is practically the same as it was for the case with free-slip walls. Boundary-layer effects do become apparent at  $171 \mu s$  when R1 begins to form a weak bifurcated structure B1, but B1 does not affect the flame until a later time. Another bifurcated structure B2 (not shown) begins to grow immediately after the incident shock reflects from the back wall, but it is quickly destroyed by a strong oblique shock coming out of the flame. Multiple reflections of oblique shocks and rarefaction waves inside the thin layer of unreacted material between the flame surface and the bottom wall prevent the formation of new bifurcated structures until about  $340 \mu s$ .

The flame remains essentially unaffected by boundary-layer phenomena until  $363 \mu s$ . By that time, R2 has passed through the flame, and a new strong bifurcated structure B3 begins to develop. When a bifurcated foot forms and grows, a recirculation region forms and grows behind it. Near the bottom wall, the flow in the recirculation region is moving towards the shock. The flame, which almost touches the bottom wall and moves with the flow behind the shock, penetrates the recirculation region. The flame approaches the shock first as a thin jet along the wall, 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 top of the foot reaches the symmetry plane (top boundary of the computational domain) and a forms a Mach reflection at the top boundary by  $424 \mu s$ .

The surface area of the flame interacting with the bifurcated shock increases, thus increasing the energy-release rate in the system. The energy release gradually increases the strength of the bifurcated shock and the Mach stem. Eventually, the temperature behind the Mach stem becomes high enough to ignite the mixture. Ignition produces several hot spots, spontaneous waves, and residual flames that grow quickly, interact with vortices, and eventually trigger a detonation D1. (*End of figure caption*)



**Figure 2.** Accelerating flame (left column), DDT, and quasi-detonation (2 right columns) in a half-channel with obstacles computed for the conditions shown by the schematic on top [8].  $d/2 = 2$  cm, the total channel length  $L = 64$  cm, and  $dx_{min} = 1/512$  cm. Times in milliseconds are shown in frame corners. The channel is filled with a stoichiometric hydrogen-air mixture at  $P_0 = 1$  atm.

A laminar flame, ignited at the left top corner of the computational domain, propagates with the velocity close to  $S_l = 298$  cm/s relative to unburned material. Hot reaction products expand and push unreacted material towards the open end of the channel. The flame front propagates with the moving flow and quickly becomes very convoluted as the flow interacts with obstacles. The increasing flame surface area results in faster energy release, thus accelerating the flow and increasing the flame speed in the laboratory frame of reference. (Caption continued on next page.)

**Figure 2.** (*Caption Continued*)

As the flame passes obstacles, it wrinkles due to the Rayleigh-Taylor (RT) instability caused by the flow acceleration and acoustic waves. The unreacted flow ahead of the flame becomes sonic by 1.4 ms, just past  $O_5$ . Noticeable shocks begin to form ahead of the flame past  $O_7$  at 1.85 ms. They reflect from obstacles and side walls, and interact with the flame triggering Richtmyer-Meshkov (RM) instabilities. Kelvin-Helmholtz (KH) instabilities develop at the flame surface when a jet of hot burned material passes through a narrow part of the channel and a shear layer forms downstream of the obstacle.

Fluid instabilities (such as Rayleigh-Taylor, Richtmyer-Meshkov, and Kelvin-Helmholtz) and flame-vortex interactions in obstacle wakes are the mechanisms responsible for increases in flame surface area, energy-release rate, and, eventually, shock strength. The elevated temperature behind shocks also contributes to the increased energy-release rate because  $S_l$  increases and shocks passing through the reaction zone release additional energy.

The average flame velocity gradually increases and reaches 800 m/s by 2.1 ms. This velocity equals about 0.8 of sound speed in the burned material, or  $0.4D_{CJ}$ , and is typical of what has been called the choking regime of flame propagation observed in experiments with obstructed channels. As the shock and the flame accelerate, the leading edge of the flame remains about 1 cm behind the leading shock, which diffracts at every obstacle and reflects from the bottom wall after each diffraction. The reflection type changes from regular to strong as the reflection point approaches the next obstacle. The resulting Mach stem becomes stronger after each diffraction, and the temperature of the hot region that forms when the Mach stem collides with an obstacle increases. At 2.100 ms, the reflection of the Mach stem from  $O_{12}$  creates a region with temperatures above 830 K. Two hot spots in this region ignite producing two small flame kernels. Then a detonation appears near one of the kernels and propagates through the unreacted material. (*End caption.*)

The newly formed detonation propagates through the gap between the flame and the obstacle into the shock-compressed material ahead of the flame. As the detonation passes around the obstacle, the lower part of the front decouples into a separated shock and a flame. The upper part of the front remains essentially undisturbed and develops detonation cells before it collides with the upper boundary. The collision creates a strong reflected shock that triggers a detonation in both the shock-compressed layer between the leading shock and the decoupled flame, and the uncompressed material. The strong detonation wave in the uncompressed material quickly develops detonation cells, collides with  $O_{13}$  at 2.125 ms, and diffracts. As the diffraction weakens the detonation wave, detonation cells grow and form an irregular two-level structure. The diffraction on  $O_{14}$  completely decouples the shock and flame by 2.164 ms, and effectively kills the detonation. A new detonation is ignited in the shock-compressed material by the collision of the Mach stem with  $O_{15}$  at 2.179 ms, but this detonation is unable to propagate through the very narrow gap between the obstacle and the flame. The leading shock and the flame remain decoupled until the Mach stem hits  $O_{16}$  and triggers a new detonation at 2.217 ms that spreads past the obstacle. This quasi-detonation regime that involves the detonation diffraction, failure, and reignition continues until the end of the channel. (*End caption.*)

### 3. Results of Current Research

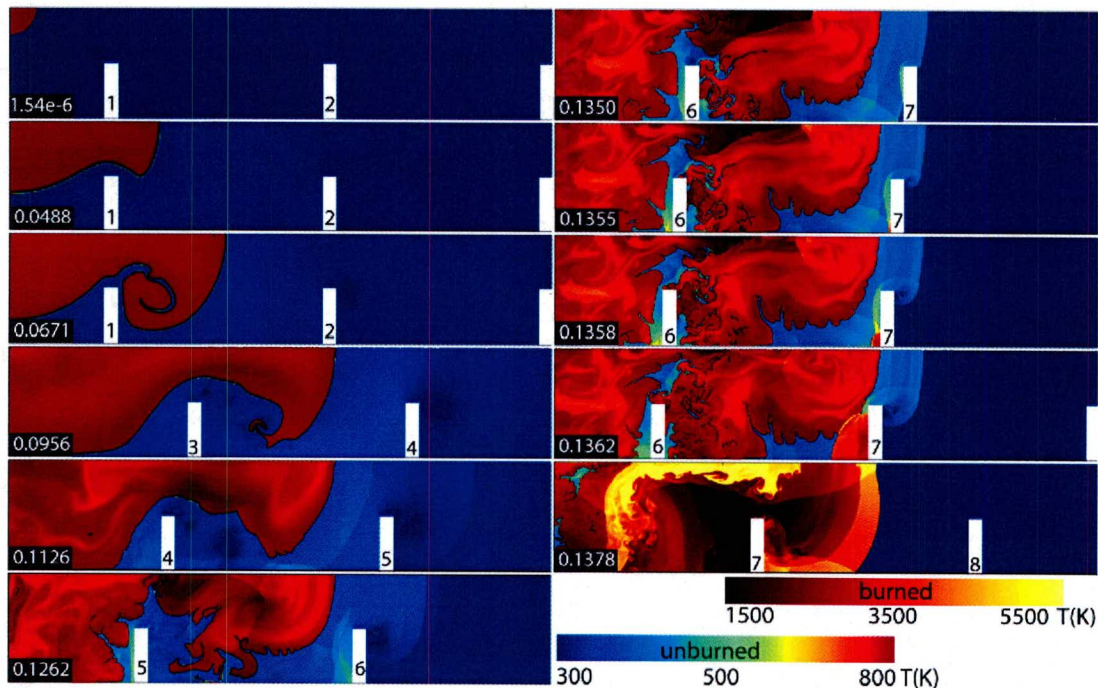
The objective of this project is to address one of the grand-challenge questions in combustion dynamics: How and under what circumstances does a flame propagating in a smooth channel accelerate to the point where there is a transition to detonation (DDT)? We are also asking: What are the specific physical mechanisms controlling this process?

Our approach is two-pronged: First, study larger channels with a defined flow blockage, and then systematically reduce the flow blockage to approach smooth-wall conditions. Second, study smooth, small-diameter channels in which there is no significant turbulence, and then systematically move to larger channels and to channels with added wall roughness, so that the additional effects of turbulence come into play.

To accomplish these objectives, we perform full multidimensional unsteady reactive-flow simulations of two- and three-dimensional systems using state-of-the-art methods for solving the fully compressible reactive flow equations, and compare these with available experimental data. The material in the rest of this section consists of brief summaries of our results in five aspects of the questions we are asking.

#### *3.1. Systematically Reducing the Obstacle Size in Channels*

The blockage ratio  $br$  of a channel is defined as the ratio of the height of an obstruction to the height of the channel. A series of simulations was performed in which the blockage ratio of the flow in the channel was systematically reduced from 0.8 to 0.05. For the large values of  $br$ , the simulations reproduced prior results of experiments and simulations showing the transition to a detonation of a small laminar flame or spark in a reactive hydrocarbon system. The flame evolution proceeds through the development of a turbulent flame, generation of shock waves forming a leading shock, development of a Mach stem (strong shock) between the leading shock and the turbulent flame, and finally reflection of the Mach stem from an obstacle. As Mach stems repeatedly reflect from obstacles, they eventually form reactive hot spots (i.e., gradients in reactivity) that can spontaneously detonate. This was shown in early work and is repeatable for the fuel tested in this project. The flame evolution and DDT from reflection is shown in Figure 3.

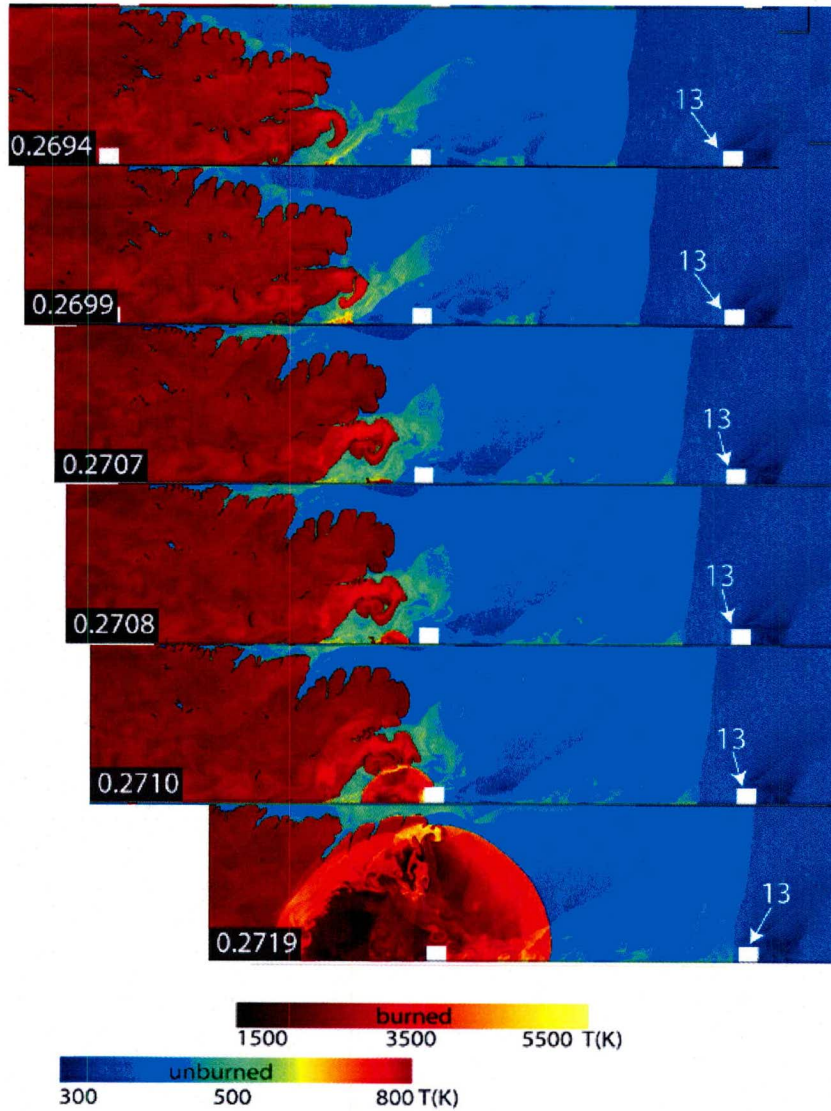


**Figure 3.** Temperature contours in burned and unburned materials, showing the evolution of an accelerating flame and the transition to a detonation in a channel with  $br = 0.5$  in an obstacle-laden channel containing stoichiometric ethylene and air.. Time is shown in milliseconds at the bottom left corner of each frame. Obstacles are numbered. There are two temperature legends, one for burned and one for unburned materials. Note the reflection at Obstacle 7, which causes a hot spot that subsequently then transitions into a detonation.

When  $br$  became very small, another route to DDT appeared. When shocks develop, they can intersect in the background unreacted flow. In some cases, the shocks and the interactions are strong enough to cause a detonation that arises spontaneously, essentially due to an intense interaction we call shock focusing. We have seen that shock focusing leading to DDT can occur in high-speed reactive material independent of any walls, boundary layers, and turbulence. This is probably related to what is called direct ignition of detonation. We believe that the shock-focusing process may help us understand the origin of DDT in purely turbulent systems with no initial shocks present. This is shown in Figure 4.

This work was published in *Combustion and Flame*, presented at the 36th International Symposium on Combustion (Seoul, Korea, August 2016), accepted for publication in the *Proceedings of the Combustion Institute*, and it was included in a paper accepted for the International Symposium on Fire and Explosion Hazards (ISFEH, Hefei, China, April

2016). In addition, portions were presented by Gabriel Goodwin (graduate student) at the Meeting of the Division of Fluid Dynamics of the American Physical Society (November, 2015).



**Figure 4.** Simulation for  $br = 0.1$  showing the transition to detonation in an obstacle-laden channel filled with stoichiometric ethylene-oxygen initially at atmospheric conditions, and for low blockage ratio. The mechanism for transition in this case is multiple shock collisions leading to energy focusing at a location near the lower boundary, between the turbulent flame and an obstacle.

### 3.2 Simulations of DDT in Small, Smooth Channels

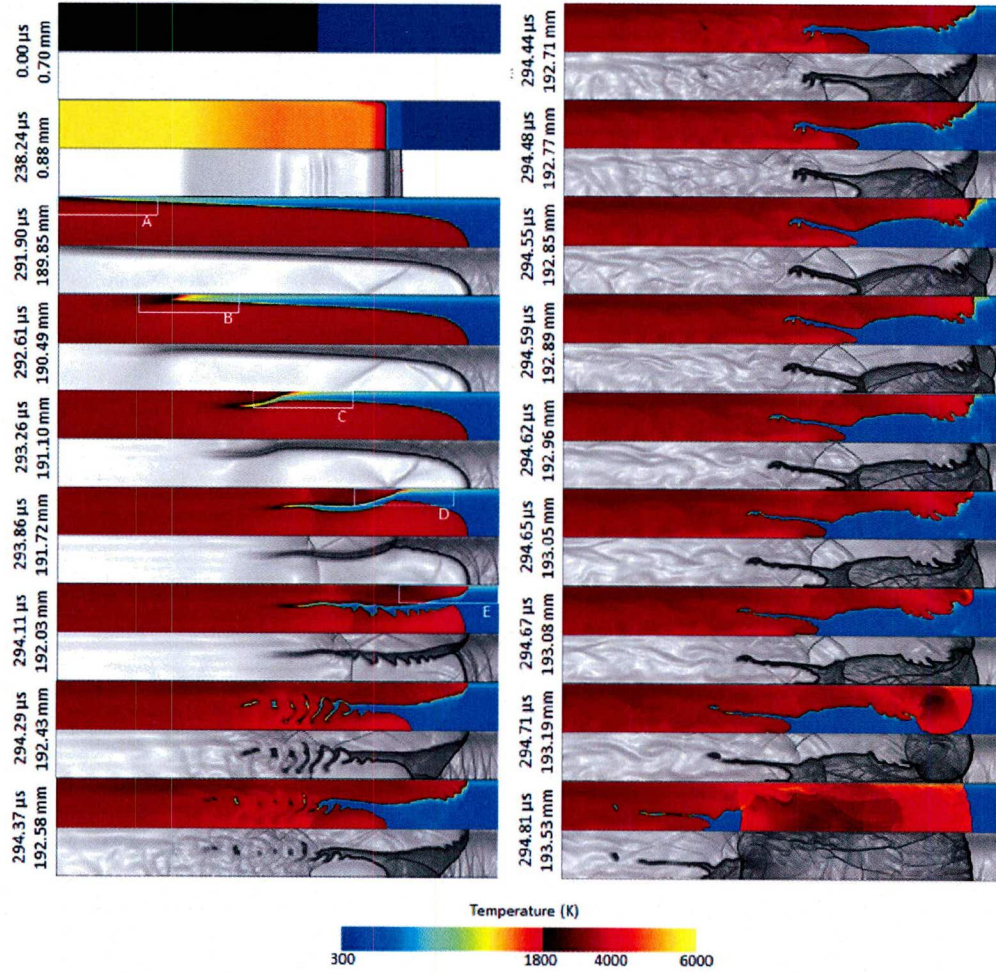
For very small completely smooth channels, the simulations have determined that the mechanism for DDT is closely connected to the development and evolution of the boundary layer. For channels with adiabatic walls, the development of hot spots in boundary layers is preceded by an instability on the flame surface, as shown in Figure 5. Subsequently, there is a combination of fluid instabilities that become important in the transition, as shown in Figure 6.



**Figure 5.** A laminar flame propagates down a smooth channel. Initially, before the hot spot is formed, and as the flow velocity increases (due to expansion and boundary-layer interactions), instabilities develop on the flame surface. This affects both the material inside the flame and the boundary layer.

In summary, the wrinkling of the flame surface combined with the high-speed flow can create weak shocks, which help produce hot spots (gradients in reactivity), which ignite spontaneously. This should be a topic of further study.

The simulations and their interpretation were presented by Alp Ozgen (former graduate student) at the Meeting of the Division of Fluid Dynamics of the American Physical Society (November, 2015), and is one of the subjects of the scholarly paper he wrote for his MS at the University of Maryland. The simulations and their interpretation has been accepted and will appear in a Special Issue of the journal *Combustion Theory and Modelling*.



**Figure 6.** Frames taken from later stages in a simulation of a detonation arising in a smooth channel from an initial small laminar flame. Each group of two frames shows temperature on top (color map below) and the related computational schlieren (density gradient map) below it. Time and position of the leading reaction front are marked on the left axis. This computation assumed an axisymmetry conditions around the centerline, so that only the top half of the computation is shown.



### 3.3. Chemical-Diffusion Models for Reactive-Fluid Simulations

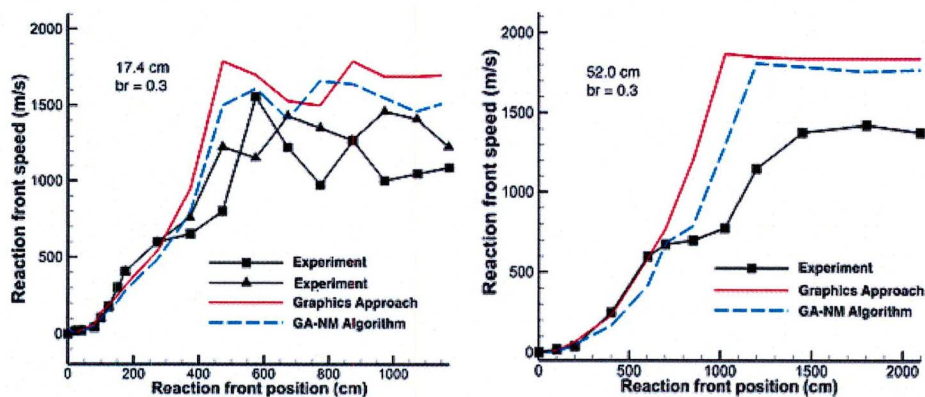
We must have fast, and sufficiently accurate models of the fundamental energy-release properties of the reactive fuel in background fluid media. Such models are important underpinnings for the research being done.

We have now developed a way to determine a reduced, but extremely useful model for the local time-varying chemical energy released as a function of time and position in a pre-specified fuel-oxidizer background. The approach is first to define a general equation for the energy release and species conversion, and ensure there are adjustable constants in that equation. The next step is to demand that when the model is inserted into a fluid computation, it reproduces the correct characteristic flame and detonation properties, such as laminar flame speed, laminar flame thickness, flame temperatures (adiabatic flame temperature and final flame temperature at constant volume), Chapman-Jouguet detonation velocity, and half-reaction thickness, given the specified background conditions.

A procedure involving a combination of a genetic algorithm with a minimization algorithm is used, such that the model finds the optimal values of reaction parameters (heat release rate, pre-exponential factor, activation energy, thermal conductivity, overall molecular weight, and ratio of specific heat at constant pressure to specific heat at constant volume) that produce the characteristic flame and detonation properties described above. This Genetic-Algorithm - Nelder Mead (GA-NM) optimization procedure has been used to find the reaction parameters for stoichiometric methane-air and ethylene-oxygen mixtures, and for mixtures of methane-air covering a broad range of fuel equivalence ratios (stoichiometries) from lean to rich conditions.

Reaction parameters obtained from this optimization procedure have been used in flame acceleration and DDT simulations of stoichiometric methane-air. For example, consider the complex problem of multidimensional flame acceleration and DDT, as discussed earlier. Figure 7 shows computed reaction front velocity as a function of position using these optimized reaction parameters and compares these to experimental measurements.

This work was presented by Alp Ozgen (former graduate student) at the Meeting of the Division of Fluid Dynamics of the American Physical Society (November, 2015), and was the primary subject of the scholarly paper he wrote for his MS at the University of Maryland in May 2016. A full paper on this work is currently being prepared for *Combustion Theory and Modelling*.

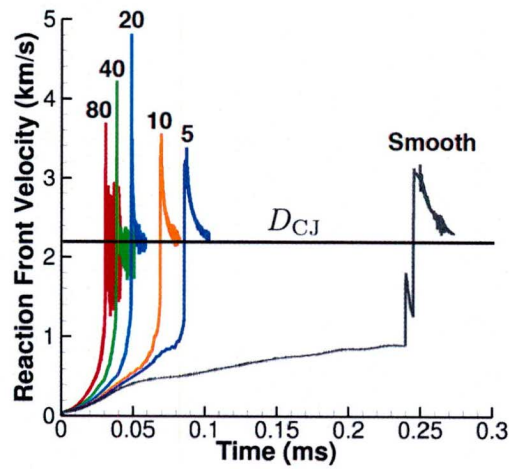


**Figure 7.** Reaction front speed as a function of reaction-front position for stoichiometric methane-air,  $br = 0.3$  for 17.4 cm (left) and 52 cm (right) channels. Comparison of experiments and simulations using two reaction-diffusion models: the newly developed GA-NM optimization procedure and a previously used “graphical” approach for finding input parameters for the model. Note the excellent agreement for smaller channels, and somewhat less agreement for larger channels. This difference for the larger channels is thought to be due to physical mechanisms playing a part in larger channels that are not accounted for by the two-dimensional simulations, and is currently under investigation.

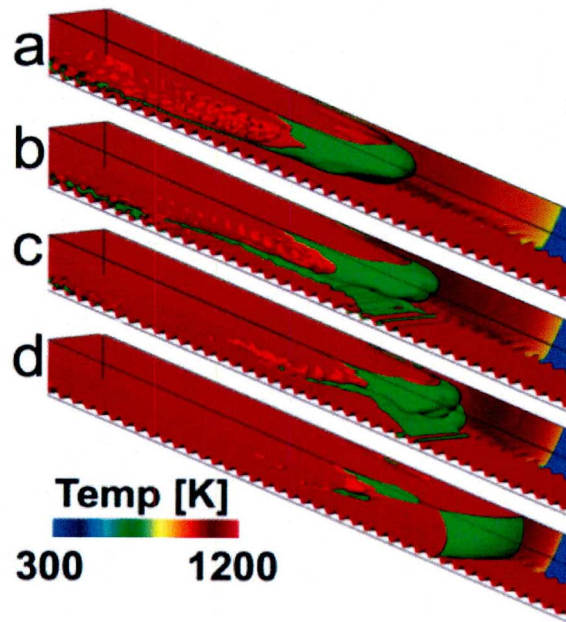
### 3.4. Effect of Surface Roughness

A series of three-dimensional simulations was used to determine the mechanism of DDT in small rectangular channels with and without surface roughness. DDT in the channel with smooth walls was produced by autoignition of boundary layers heated by viscous dissipation. Roughness on the channel walls produce shock reflections that create turbulence and intensify turbulence as the gas flows around the rough walls. The result is a pressure increase near the flame. In addition, intense shear, produced by gas flowing between the rough surfaces, produces a boundary layer-like region and locally heats unburned material. These conspiring effects lead to a situation where autoignition can occur and there is a transition to detonation. The DDT run-up distance is up to 15 times shorter in the rough-walled channels compared to the smooth-walled channel as a result of enhanced flame acceleration. A summary of the results is shown in Figure 8 and a series of frames from a typical calculation is shown in Figure 9.

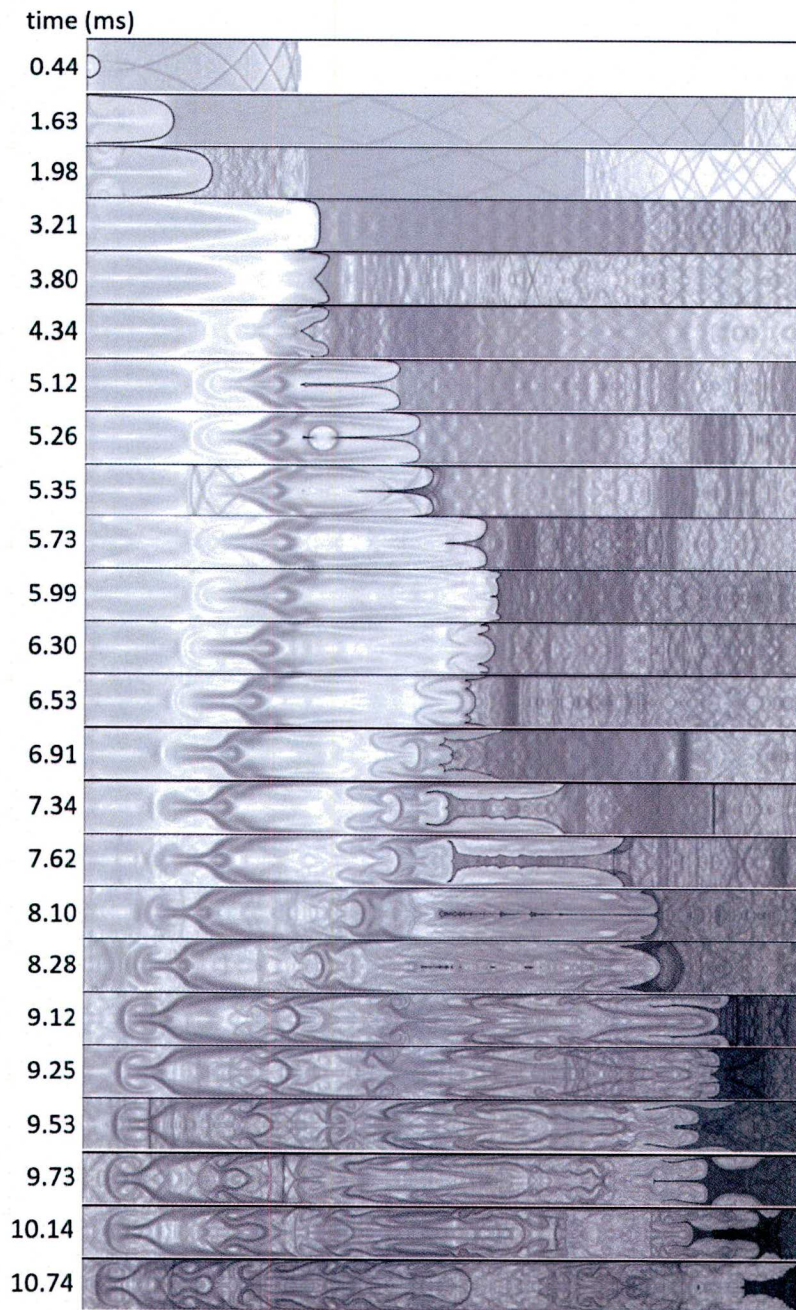
This work is now being prepared now as a full paper for *Combustion and Flame*. Part of the work appeared in the invited article for *Combustion Theory and Modelling* referenced above.



**Figure 8.** Summary of time to DDT for the smooth wall compared to roughness of various heights over the bottom surface. Roughness heights (5, 10, 20, 40, 80) are in microns.  $D_{CJ}$  is the equilibrium detonation velocity.



**Figure 9.** Frames from a three-dimensional simulation of flame acceleration and DDT in a rough-walled channel. The channel (240 mm x 240 mm x 5 cm) is filled with a mixture of ethylene and O<sub>2</sub> at STP. Open boundary at the right. One quarter of the channel shown. (a) Rough walls generate turbulence. Flame (green) accelerates as it propagates down the channel. (b) DDT in the boundary layer near the back wall. (c,d) The newly formed detonation overtakes the flame and consumes reactants.



**Figure 10.** Sequence of numerical schlieren images showing the evolution of premixed stoichiometric hydrogen-air flame and strong pressure waves interacting with the flames in a 4 cm × 56 cm closed channel. Time (ms) is given on the left side of each frame. Only half of the channel was simulated and each time instance is mirrored about the symmetry line (centerline).

### 3.5. Turbulence through Flame-Acoustic Interactions in Closed Channels

In this work, we determined a route to turbulence proceeding through acoustic interactions with laminar flames ignited in a large enclosed channel. This process starts with the formation of the standard a tulip-flame structure, which developed into a distorted tulip flame. Then acoustic interactions with these flames lead to flame-surface instabilities. Eventually, for a long enough channel, shocks form and DDT may develop. Figure 10 is taken from one of the calculations and is explained below.

The numerical simulations reproduced major experimental observations of tulip and distorted tulip flames. The flame develops a usual tulip flame (defined as a flame with its center part concaved toward burned region) and develops a deep cusp (5.12 ms) due to interactions between flame, fluid motion and and boundary layer in the early stages. The initial contact of the flame front with the sidewalls generates strong acoustic waves (1.98 ms), which were demonstrated to be expansion waves. The collapse of the tulip cusp produces another strong expansion wave (5.26 and 5.35 ms). A distorted tulip flame forms after 5.90 ms and appear as additional cusps on the lips of the original tulip flame (see 5.99 ms). Then the distorted tulip flame develops a double-cusped, concave flame front (6.91 and 7.34 ms). By this time, the pressure waves are amplified, and eventually generate shock waves.

The pressure waves interact with the flame, and thus the flame front is dramatically distorted again after 7.92 ms (8.28 and 9.12 ms). A long, narrow unburned region forms in the center region of the tube as the second distorted flame starts to form (8.10 ms). The collapse of the cusp generates additional expansion waves (8.28 ms). These waves coalesce with the prior waves to form stronger pressure waves. The flame is distorted for the third time at about 9.18 ms after a shock pass through it from unburned to burned side (see flames at 9.25 and 9.53 ms). The pressure waves continues to interact with the flame and lead to more flame distortions and turbulences as the flame approaches the right wall (9.73 and 10.14 ms).

The simulations showed that a flame front propagating in a closed channel can develop very complex shapes, including a hemispherical, curved, tulip, distorted tulip, highly corrugated and turbulent flames. Rayleigh-Taylor (RT) instability arises from the generation of vorticity through baroclinic effects when a curved material interface is exposed to a pressure gradient and there is a misalignment between pressure and density gradients. Since pressure waves are so prominent, the RT instability can be significant. A time scale and

pressure wave analysis of the results, combined with a linear theory to give the growth rate of the RT instability, showed that the RT instability is a primary cause for the initiation of distorted tulip flames. When shock waves are generated, Richtmyer-Meshkov (RM) instabilities arise due to their interaction with the flame front. Evidence of Kelvin-Helmholtz (KH) instabilities were also observed along the flame surface due to the interaction between flame front, strong acoustic waves and shock waves (7.62 and 8.10 ms).

Part of this work was published in *Combustion and Flame* and presented at the 25th International Colloquium on the Dynamics of Explosions and Energetic Systems in Leeds, UK August 2015. Another part was presented at the 36th International Symposium on Combustion (Seoul, Korea, August 2016) and accepted for publication in *Proceedings of the Combustion Institute*.

#### 4. Technical Publications and Presentations – Output of Research

##### 4.1 Refereed Journal Articles

*Formation and Evolution of a Distorted Tulip Flame*, H. Xiao, R.W. Houim, and E.S. Oran *Combustion and Flame*, 162, 4084–4101, 2015.

*Large-Scale Experiments and Absolute Detonability of Methane/Air Mixtures*, E.S. Oran, V.N. Gamezo and R.K. Zipf, Jr., *Combustion Science and Technology*, 187, 324–341, 2015.

*Understanding Explosions – From Catastrophic Accidents to Creation of the Universe*, E.S. Oran, *Proceedings of the Combustion Institute*, 35, 1–35, 2015.

*Effect of Decreasing Blockage Ratio on DDT in Small Channels with Obstacles*, G.B. Goodwin, R.W. Houim, E.S. Oran, *Combustion and Flame*, 173, 16–26, 2016.

*The Role of Spontaneous Waves in the Deflagration-to-Detonation Transition in Submillimetre Channels*, R.W. Houim, A. Ozgen and E.S. Oran, *Combustion Theory and Modelling*, 20, 1068–1087, 2016.

*Effects of Pressure Waves on the Stability of Flames Propagating in Tubes*, H. Xiao, R.W. Houim, E.S. Oran. *Proceedings of the Combustion Institute* 36, <http://dx.doi.org/10.1016/j.proci.2016.06.126>, 2017.

*Shock Transition to Detonation in Channels with Obstacles*, G.B. Goodwin, R.W. Houim, E.S. Oran, *Proceedings of the Combustion Institute*, 2017,

<http://dx.doi.org/10.1016/j.proci.2016.06.160>.

*Optimization of Chemical-Diffusive Models for Deflagration-to-Detonation Transition Calculations*, C.R. Kaplan, A. Ozgen, E.S. Oran, in preparation for *Combustion Theory and Modeling*.

#### 4.2 Refereed Conference Proceedings

*More on Mechanisms of DDT in Reactive Gases*, E.S. Oran, *Proceedings of the Eighth International Seminar on Fire and Explosion Hazards (ISFEH8)*, to appear, 2017.

*Formation and Evolution of Distorted Tulip Flames*, H. Xiao, R.W. Houim, E.S. Oran, J. Sun, *Proceedings of the 25th International Colloquium on the Dynamics of Explosions and Energetic Systems*, Leeds University, 2015.

#### 4.3 Invited Presentations

The Reactive Flow of Ideas, Fluid Dynamics Prize and the Otto Laporte Lecture, E.S. Oran, American Physical Society, Division of Fluid Dynamics, Pittsburgh PA, November 2013.

Turbulence and Energetic Reactive Flows, E.S. Oran, Syracuse University, Syracuse NY, March 2014.

Turbulence and Energetic Reactive Flows, E.S. Oran, Northwestern University, Xian, China, April 2014.

Turbulence and Energetic Reactive Flows, E.S. Oran, Institute of Mechanics, Academy of Sciences, Beijing, China, April 2014.

Effects of Turbulence and Scale on Flame Acceleration, Detonations, and DDT Experiments at Lake Lynn Laboratories, Beijing Institute of Technology, Beijing China, April 2014.

Turbulence and Energetic Reactive Flows, E.S. Oran, Beijing Institute of Technology, Beijing China, April 2014.

Turbulence and Energetic Reactive Flows, E.S. Oran, 34th Annual Combustion Meeting of the Department of Energy, Potomac MD, May 2014.

Numerical Simulations of Industrial Explosions Discussions of the Impossible and Improbable, E.S. Oran, Tenth international Symposium on Hazards, Prevention and Mitigation of Industrial Explosions, Bergen, Norway, June 2014.

Understanding Explosions From Catastrophic Accidents to the Creation of the Universe, E.S. Oran, Hoyt C. Hottel Lecture, 35th International Symposium on Combustion, San Francisco CA, August 2014.

Turbulence and Transition in Energetic Reactive Flows, E.S. Oran, Institute for Physical Sciences and Technology, University of Maryland, December 2014.

Understanding Explosions – From Catastrophic Accidents to the Creation of the Universe, Institute National Scientifique Appliquée, Rouen, France, April 2015.

Turbulence, Noise, and Predictability – Basic Issues for High-Speed Reactive Flows, E.S. Oran, Statistical Physics Seminar, Institute of Physical Sciences and Technology, University of Maryland, September 2015.

Turbulence and Energetic Reactive Flows, E.S. Oran, William Maxwell Reed Seminar, University of Kentucky, Lexington KY, March 2016.

Premixed Flame Propagation in Hydrogen Explosions, J. Sun, H. Xiao, 11th International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosion, Dalian, China, July 2016.

Understanding Newly Discovered Flames, H. Xiao, University of New South Wales, Australia, August 2016.

Combustion Transitions, E.S. Oran, Workshop on Physics of Turbulent Combustion Nordita, Stockholm September 28, 2016.

The Nature of Flames and Detonations, E.S. Oran, Symposium to honour the 90th year of Derek Bradley, Leeds University, September 2016.

Pressure Gain Combustion in Microchannels: Flame Acceleration and Transition to Detonation, R. Houim, 1st International Workshop on Near Limit Flames, Boston, MA, July 2017.

#### *4.4 Contributed Presentations*

Formation and Evolution of Distorted Tulip Flames, H. Xiao, R.W. Houim, E.S. Oran 25th International Colloquium on the Dynamics of Explosions and Energetic Systems, Leeds, UK August, 2015.

Flame Acceleration and Transition to Detonation in Channels, G. Goodwin, R.W. Houim, and E.S. Oran, 68th Annual Meeting of the American Physical Society Division of Fluid Dynamics, Boston, MA, November 2015.



Optimizing Simplified One-Step Chemical Models for High Speed Reacting Flows, A. Ozgen, R.W. Houim, and E.S. Oran, 68th Annual Meeting of the American Physical Society Division of Fluid Dynamics, Boston, MA, November 2015.

(More on) Mechanisms of DDT in Reactive Gases, E.S. Oran, 8th International Seminar on Fire and Explosion Hazards, (ISFEH8) Hefei, Anhui, China, April 2016.

Flame Acceleration and Transition to Detonation in Channels with Decreasing Blockage Ratio, G. Goodwin, R. Houim, and E. Oran, 36th International Symposium on Combustion, Seoul, Korea, August 2016.

Effects of Pressure Waves on the Stability of Flames Propagating in Tubes, H. Xiao, R. Houim, E. Oran, 36th International Symposium on Combustion, Seoul, Korea, August 2016.

Shock-Flame Complexes: Transitional and Steady States, E.S. Oran, I24th International Congress of Theoretical and Applied Mechanics, Montreal, Canada, August 2016.

#### *4.5 Technical Reports*

Optimizing Simplified One-Step Chemical-Diffusive Models for Deflagration-to-Detonation Transition Calculations, Scholarly paper by Alp Ozgen, for an MS degree in Aerospace Engineering, University of Maryland, May 2016.

#### *4.6 Related Sponsored Work*

Alpha Foundation for Research in Coal Mine Safety, for scaling laws for DDT events in laboratory sized phenomena to large coal mine-sized tunnels.

National Institute of Occupational Safety and Health Pittsburgh Research Laboratory for study of dust explosions.

Shell research (Britain) – Study of DDT in large-scale explosions.

## **5. Summary and Conclusions**

We have carried out a program that allowed us to hone in on the mechanism for flame acceleration and the transition to detonation in smooth channels by approaching the problem from different directions of channel size and smoothness. In the process, we have found a mechanism for DDT that helps explain what is observed in highly turbulent, unconfined

systems as well as in confined systems. In addition, we have developed a new approach to finding energy-release models for these types of complex, energetic reacting flows.

We have answered part, but not all, of the grand challenge question. We have observed and explained DDT in small smooth channels with adiabatic walls: DDT always starts with autoignition (hot spot) in the boundary layer, even though the subsequent development to the final stage might be different. In all cases the autoignition produces a hot spot that evolves into a spontaneous wave. As this wave travels, it relaxes to a detonation. For cases in which the spontaneous wave does not directly produce a detonation, it produces shock-shock and shock-flame interactions that do lead to more intense hot spots that do lead to detonations.

This work has brought out two controversial issues. The first concerns the mechanism we see for DDT in a smooth channel, which opposes that maintained by members of the community. They say that the flame tip accelerates, that is, the flame front itself becomes a detonation. We attempted to reproduce their computations and found that they are numerically under-resolved.

The second controversy concerns the energy-release mechanism that represents the chemical reactions and diffusion processes. Our point is that there is little use in using an incredibly expensive chemical-diffusive mechanism (hundreds of species, thousands of chemical reaction rates) when most of the input parameters in these models are guesses, at best, and certainly incorrect in high-pressure, high-temperature, shock-laden flows. Therefore we developed a simplified parametric model that works because it deposits the right amount of energy in the right location at the right time. Much of the combustion and energy community has moved in the direction of more and more complex reaction mechanisms, which might be reasonable for gases at low pressures, low temperatures, and without shocks.

Both of these controversial issues are defensible, although the most important to the community is probably the chemical-diffusive model.

## 6. References

1. E.S. Oran and V.N. Gamezo, *Origins of the deflagration-to-detonation transition in gas-phase combustion*, *Combustion and Flame* 148 (2007) 4–47.
2. G. Ciccarelli and S. Dorofeev, *Flame acceleration and transition to detonation in ducts*, *Progress in Energy and Combustion Science* 34 (2008) 499–550.

3. V.N. Gamezo, T. Ogawa, and E.S. Oran, *Flame acceleration and DDT in channels with obstacles: Effect of obstacle spacing*, *Combustion and Flame* 155 (2008). 302–315.
4. M. Kuznetsov, G. Ciccarelli, S. Dorofeev, V. Alekseev, Yu. Yankin, and T.H. Kim, *DDT in methane-air mixtures*, *Shock Waves* 12 (2002) 215–220.
5. M. Kuznetsov, V. Alekseev, I. Matsukov, and S. Dorofeev, *DDT in a smooth tube filled with a hydrogen-oxygen mixture*, *Shock Waves* 14 (2005) 205–215.
6. E.S. Oran and J.P. Boris, *Numerical Simulation of Reactive Flow*, Second Edition, New York: Cambridge University Press, 2001.
7. A.M. Khokhlov, E.S. Oran, and G.O. Thomas, *Numerical simulation of deflagration-to-detonation transition: The role of shock-flame interactions in turbulent flames*, *Combustion and Flame* 117 (1999) 323–339.
8. V.N. Gamezo, T. Ogawa, and E.S. Oran, *Numerical simulations of flame propagation and DDT in obstructed channels filled with hydrogen-air mixture*, *Proceedings of the Combustion Institute* 31 (2007) 2463–2471.
9. A.Y. Poludnenko, T.A. Gardiner, and E.S. Oran, *Spontaneous transition of turbulent flames to detonations in unconfined media*, *Physical Review Letters* 107 (2011) 054501.
10. A.M. Khokhlov, E.S. Oran, A.Yu. Chtchelkanova, and J.C. Wheeler, *Interaction of a shock with a sinusoidally perturbed flame*, *Combustion and Flame* 117 (1999) 99–116.
11. A.M. Khokhlov and E.S. Oran, *Numerical simulation of detonation initiation in a flame brush: The role of hot spots*, *Combustion and Flame* 119 (1999) 400–416.
12. V.N. Gamezo, A.M. Khokhlov, and E.S. Oran, *The influence of shock bifurcations on shock-flame interactions and DDT*, *Combustion and Flame* 126 (2001) 1810–1826.
13. V.N. Gamezo, A.M. Khokhlov, and E.S. Oran, *Effects of wakes on shock-flame interactions and deflagration-to-detonation transition*, *Proceedings of the Combustion Institute* 29 (2002) 2803–2808.
14. V.N. Gamezo, E.S. Oran, and A.M. Khokhlov, *Three-dimensional reactive shock bifurcations*, *Proceedings of the Combustion Institute* 30 (2005) 1841–1847.
15. T. Ogawa, V.N. Gamezo, and E.S. Oran, *Flame acceleration and transition to detonation in an array of square obstacles*, In *Proceedings of the Eighth International Symposium on Hazards, Prevention, and Mitigation of Industrial Explosions* Yokohama, Japan, Sept. 5-10, 2010.
16. D.A. Kessler, V.N. Gamezo and E.S. Oran, *Simulations of flame acceleration and deflagration-to-detonation transitions in methane-air systems*, *Combustion and Flame*

- 157 (2010) 2063–2077.
17. A.Y. Poludnenko and E.S. Oran, *The interaction of high-speed turbulence with flames: Global properties and internal flame structure*, *Combustion and Flame* 157 (2010) 995–1011.
  18. A.Y. Poludnenko, and E.S. Oran, *The interaction of high-speed turbulence with flames: Turbulent flame speed*, *Combustion and Flame* 158 (2011) 301–326.
  18. P.E. Hamlington, A.Y. Poludnenko, E.S. Oran, *Interactions between turbulence and flames in premixed reacting flows*, *Physics of Fluids* 23 (2011). 125111.
  19. M.F. Ivanov, A.D. Kiverin, and M.A. Liberman. *Hydrogen-oxygen flame acceleration and transition to detonation in channels with no-slip walls for a detailed chemical reaction model*, *Physical Review E* 83 (2011) 056313.
  20. B.D. Taylor, D.A. Kessler, V.N. Gamezo, and E.S. Oran. *Numerical simulations of hydrogen detonations with detailed chemical kinetics*, *Proceedings of the Combustion Institute*, 34, (2013) 2009-2016.