Flame Acceleration, DDT, and Hydrogen in Channels

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Proposed Hydrogen Fuel Station

Fuel leakages could lead to flames and even detonations ...

(Shimizu Corporation, 2005-)
Deflagration and Detonation

Deflagration

- Window glass shatters

Detonation

- Concrete shatters
- Brick shears apart
- Lung damage
- Eardrum rupture

A flame ignited in leaked H₂ gas could undergo a deflagration-to-detonation transition!
Focus of Recent Research

Answer the question:
How confidently ... qualitatively or quantitatively ... can we compute hydrogen combustion from ignition, to flame acceleration, and even to DDT?

This Involves:

-- Developing and test low-cost, low-order chemical-diffusive models

-- Developing and test high-order methods with AMR

-- Testing performance of multidimensional, reactive numerical models
H₂-Air Mixture Ignited in a Channel with Obstacles

Movie will show how ...

... starting with spark ignition in enclosures containing combustible mixures, turbulent flames develop and produce shock waves. This leads to the formation of unsteady shock-flame complexes and detonations.
Channels with Obstacles

Channels filled with stoichiometric H$_2$-Air

$d/2 = 1, 2, 4, \text{ or } 8 \text{ cm};$ Constant blockage ratio

Smooth or spark ignition; Constant input energy

[Diagram showing channels with obstacles and stoichiometric H$_2$-Air]
The initially laminar flame moves slowly into the unreacted material (to the right).

Obstacles perturb the flow, which then interacts with and distort the flame, so that the flame becomes turbulent.
Shock Wave Formation

The turbulent flame generates compression waves, which eventually coalesce to form a shock in front of the flame.

The shock is continuously strengthened by compression waves coming from behind.
Transition to Detonation

The shock reflects from an obstacle ... creates a hot spot ... which becomes a spontaneous wave ...

- A detonation wave results that *may or may not* survive.
Computational Result
Detonation Wave Propagation

Quasi-detonation for $d = 4$ and $8$ cm

The detonation diffracts from the obstacle, and the shock and flame separate.

Detonation wave

Flame

Detonation decays to deflagration.

This phenomenon repeats.

Detonation occurs again.

2.301 ms  2.313 ms  2.328 ms

2.340 ms  2.369 ms  2.375E ms
For large enough channels, the detonation successfully propagates over the obstacle.

The detonation is partially extinguished, but quickly recovers.
Regimes of Flame Propagation

1. Slow deflagrations
   subsonic

2. Fast deflagrations (“choking”)
   \[ \frac{1}{3} - \frac{1}{2} D_{\text{CJ}}, \leq c_s \text{ in burned gas} \]
   Flame decoupled from leading shock, spreads through molecular or turbulent diffusion and convection.

3. Quasi-detonations
   \[ < D_{\text{CJ}} \]
   Shock & flame coupled some sometimes when reaction triggered by shock compression. Sometimes, shock and flame decoupled as detonation defracts over obstacles. Observed when width of unobstructed part of channel > few times l. Propagation velocity increases with d/l, and reaches \( D_{\text{CJ}} \) when propagation becomes independent of diffraction effects.

4. Detonations
   \( D_{\text{CJ}} \)
H$_2$-Air Mixture Ignited in a Channel with Obstacles
Two Modes of Ignition

Smooth Flame Ignition

Spark Ignition

Initial development appears quite different: Immediate effects of shocks apparent for spark ignition. Time to DDT less for spark ignition (0.61 ms from 0.76 ms) Location is essentially the same.
Experimental Tests

- DDT in a channel with obstacles
  - For example, piping space
  - The same conditions as computations

- Conducted by Andrej Teodorczyk
  Warsaw University of Technology
The distance to DDT is proportional to \( d^2 \)
Cases Considered for H₂-Air Channels

Variations on:
Form of ignition (smooth vs spark)
Channel height \((d/2)\)
Blockage ratio
Obstacle spacing \((S)\)
Obstacle symmetry (top and bottom)
Dimensionality (3D vs 2D)
***********
Stoichiometry
Stochasticity
...
Back to the Basics ....

Chemical model
   Effects of variable stoichiometry

Even more complex geometries

Why do simulations “work” ..?

Effects of non-Kolmogorov turbulence

Stochasticity
THE PHYSICAL MODEL

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \]

\[ \frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) + \nabla P + \nabla \cdot \hat{\tau} = 0 \]

\[ \frac{\partial E}{\partial t} + \nabla \cdot ((E + P) \mathbf{U}) + \nabla \cdot (\mathbf{U} \cdot \hat{\tau}) + \nabla \cdot (K \nabla T) = 0 \]

\[ \frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho Y \mathbf{U}) + \nabla \cdot (\rho D \nabla Y) - \rho \dot{\omega} = 0 \]

\[ \hat{\tau} = \rho \nu \left( \frac{2}{3} (\nabla \cdot \mathbf{U}) \hat{I} - (\nabla \mathbf{U}) - \nabla \mathbf{U} \right) \]

\[ P = \frac{\rho R T}{M} \]

\[ E = \frac{P}{(\gamma - 1)} + \frac{\rho U^2}{2} \]

\[ \frac{dY}{dt} \equiv \dot{w} = -A \rho Y \exp \left( -\frac{Q}{RT} \right) \]

\[ \nu = \nu_0 \frac{T^n}{\rho} \]

\[ D = D_0 \frac{T^n}{\rho} \]

\[ \frac{K}{\rho C_p} = \kappa_0 \frac{T^n}{\rho} \]

\[ Le = \frac{K}{\rho C_p D} = \frac{\kappa_0}{D_0} \]

\[ Pr = \frac{\rho C_p \nu}{K} = \frac{\nu_0}{\kappa_0} \]

\[ Sc = \frac{\nu}{D} = \frac{\nu_0}{D_0} \]
Material, Chemistry, and Reaction Wave Parameters
Stoichiometric Hydrogen-Air

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$T_0$</td>
<td>293 K</td>
<td>Initial temperature</td>
</tr>
<tr>
<td>$P_0$</td>
<td>1 atm</td>
<td>Initial pressure</td>
</tr>
<tr>
<td>$\rho_0$</td>
<td>$8.7345 \times 10^{-4}$ g/cm$^3$</td>
<td>Initial density</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.17</td>
<td>Adiabatic index</td>
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<tr>
<td>$M$</td>
<td>21 g/mol</td>
<td>Molecular weight</td>
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<tr>
<td>$A$</td>
<td>$6.85 \times 10^{12}$ cm$^3$/g-s</td>
<td>Pre-exponential factor</td>
</tr>
<tr>
<td>$E_a (= Q)$</td>
<td>$46.37 , R_0$</td>
<td>Activation energy</td>
</tr>
<tr>
<td>$q$</td>
<td>$43.28 , R_0/M$</td>
<td>Chemical energy release</td>
</tr>
<tr>
<td>$\nu_0 = \kappa_0 = D_0$</td>
<td>$2.9 \times 10^{-5}$ g/s-cm-K$^{0.7}$</td>
<td>Transport constants</td>
</tr>
<tr>
<td><strong>Output</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$S_l$</td>
<td>298 cm/s</td>
<td>Laminar flame speed</td>
</tr>
<tr>
<td>$T_b$</td>
<td>$7.289 , T_0$</td>
<td>Post-flame temperature</td>
</tr>
<tr>
<td>$\rho_b$</td>
<td>$0.1372 , \rho_0$</td>
<td>Post-flame density</td>
</tr>
<tr>
<td>$x_l$</td>
<td>0.035 cm</td>
<td>Laminar flame thickness</td>
</tr>
<tr>
<td>$D_{CJ}$</td>
<td>$1.993 \times 10^5$ cm/s</td>
<td>CJ detonation velocity</td>
</tr>
<tr>
<td>$P_{ZND}$</td>
<td>$31.47 , P_0$</td>
<td>Post-shock pressure</td>
</tr>
<tr>
<td>$P_{CJ}$</td>
<td>$16.24 , P_0$</td>
<td>Pressure at CJ point</td>
</tr>
<tr>
<td>$T_{ZND}$</td>
<td>$3.457 , T_0$</td>
<td>Post-shock temperature</td>
</tr>
<tr>
<td>$T_{CJ}$</td>
<td>$9.010 , T_0$</td>
<td>Temperature at CJ point</td>
</tr>
<tr>
<td>$\rho_{ZND}$</td>
<td>$9.104 , \rho_0$</td>
<td>Post-shock density</td>
</tr>
<tr>
<td>$\rho_{CJ}$</td>
<td>$1.802 , \rho_0$</td>
<td>Density at CJ point</td>
</tr>
<tr>
<td>$x_d$</td>
<td>$0.01927$ cm</td>
<td>1D half-reaction thickness</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>1–2 cm</td>
<td>Detonation cell size</td>
</tr>
</tbody>
</table>
A two-dimensional calculation of a propagating detonation, with enough resolution, produces reasonable detonation cell structure.

Background: 1 atm, 293 K
Stoichiometry H₂-air
Minimum \( dx = \frac{1}{2048} \) cm

Two-level detonation cell structure,
\[ \lambda = 1 - 2 \text{ cm} \]
Hot-Spot Ignition in Stoichiometric Hydrogen-Air

Consider three different gradients. \( dx = 0.016 \text{ cm} \), uniform mesh.

Hot spot created by assuming adiabatic mixing between hot burned and cold unburned gases.

\[ C \text{ is concentration (mass fraction of unburned material)} \]

\[ \frac{dC}{dx} = \frac{0.4}{R} \quad \text{and} \quad \frac{dC}{dy} = 2 \frac{dC}{dx} \]

Result is an elliptical distribution.

At the center,

\[ C = 0.6 \quad T = 1029 \text{ K} \]

\( R = 7 \)

Gradient too steep to ignite a detonation.
Result is a decoupled flame and a shock

\( R = 8 \)

Detonation appears in the \( y \)-direction

\( R = 10 \)

Detonation appears in both directions
Case 1 -- 
Ignition in gradient leaves a shock and a flame

Case 2 -- 
Ignition in gradient - intermediate case

Case 3 
Ignition in gradient produces a detonation

Background: unshocked: 1 atm, 293 K. Each frame is 8.2 cm x 8.2 cm. dx = 0.016 cm.
An Array of Obstacles

- Array of 1 cm x 1 cm square obstacles
- H₂-Air background
- Staggered layout
DDT in an Array of Obstacles

1. Initial flame

2. The flame becomes turbulent.

3. Shock wave formation

4. DDT: shock reflection from obstacles
Array of Obstacles

\[ S = 1 \text{ cm}, \quad w = 1 \text{ cm} \]  
(staggered)

\[ S = 1 \text{ cm}, \quad w = 4 \text{ cm} \]  
(symmetric)

Different size and layout
Flame Propagation and DDT in Channel with Obstacles
2D and 3D Calculations - Summary

Two Effects to Note:
- Ignition of Hot Spots
- Effect of Scale

System has to be big enough to sustain DDT
These are related ...

DDT = First successful hot-spot transition

Choking flame: 1 cm
Quasi-detonation: 2, 4 cm
Detonation: 8 cm

And now we have experiments (Teordorczyk, 2006)
Thoughts on the “Mysterious” Agreement ...

Richtmyer-Meshkov interactions are a source of turbulence in compressible, high-speed flows with repeated shock-flame interactions.

2D and 3D RM interactions have very similar growth rates and amplitudes -- both qualitatively and quantitatively -- in the linear regime, and differ only slightly well into the nonlinear regime.

RM can be the major source of turbulence, and when this is the case, all scales are populated simultaneously.

This gives us a clue as to why 2D and 3D simulations of high-speed deflagrations have certain similar properties.
Where do we go from here?

Calibration with experiments

Chemical model
  Effects of variable stoichiometry
  Other detonable materials

Even more “difficult” geometries

Why do simulations “work” ..?
  Effects of non-Kolmogorov turbulence

Stochasticity