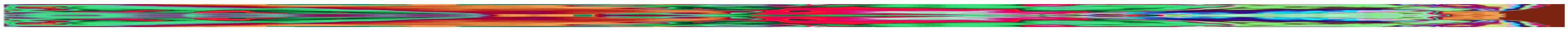
Flame Acceleration, DDT, and Hydrogen in Channels



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Sponsored by:

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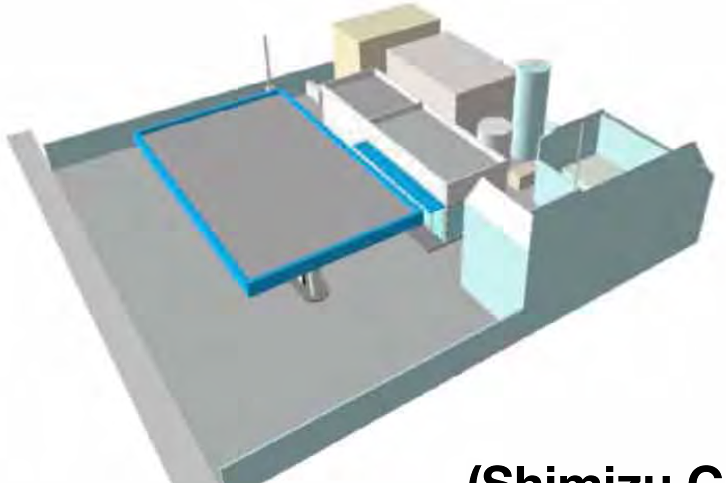
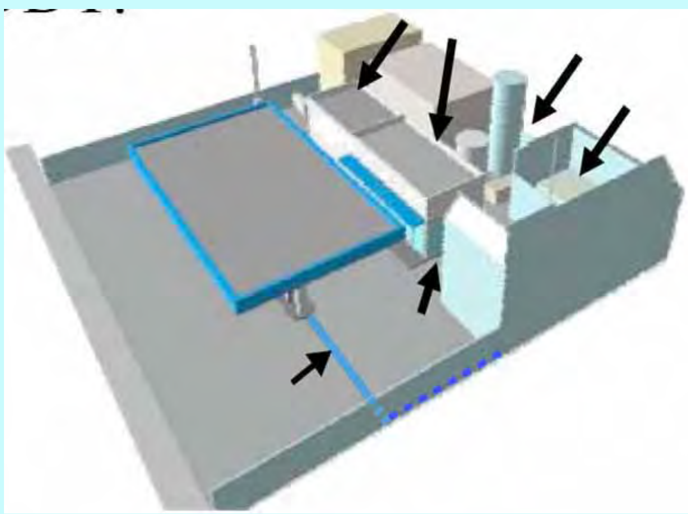
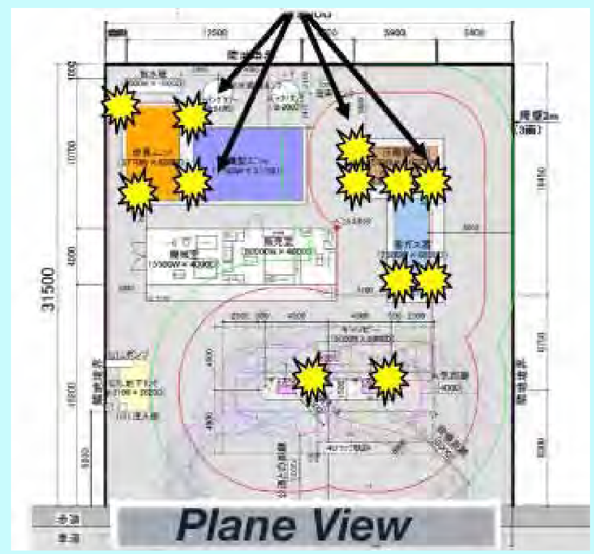
Proposed Hydrogen Fuel Station



(Shimizu Corporation, 2005-)

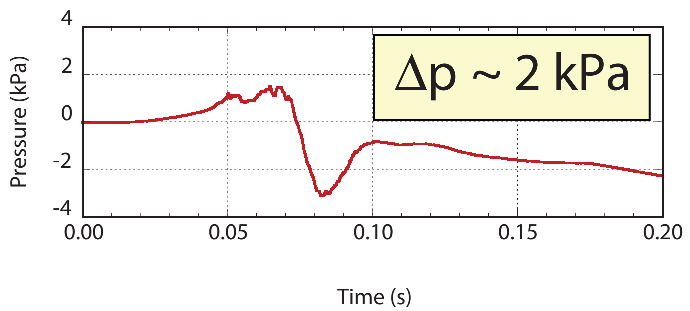
Fuel leakages could lead to flames and even detonations ...



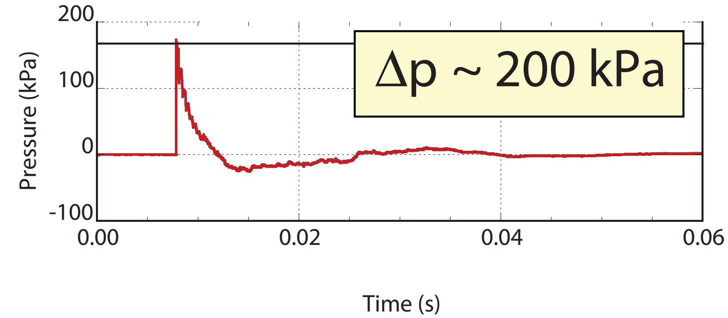


Deflagration and Detonation

Deflagration



Detonation



Pressure histories at 4m away from the ignition point for 5.27m^3 of a H_2-air mixture

- **Window glass shatters**

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

A flame ignited in leaked H_2 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:

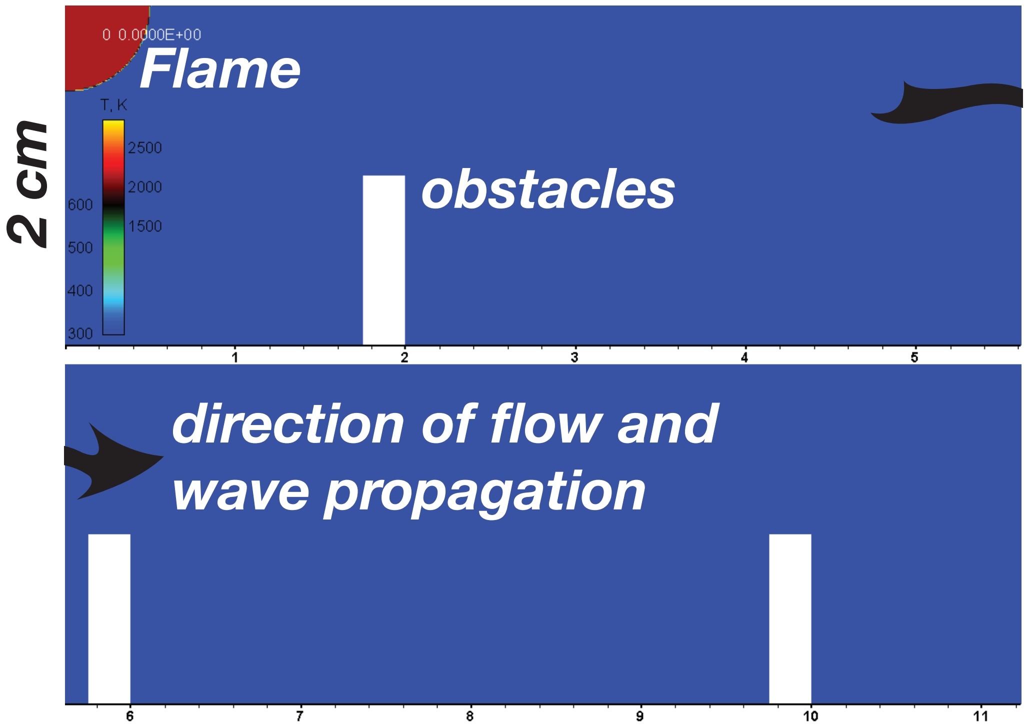
-- Developing and test low-cost, low-order chemical-diffusive models

-- Developing and test high-order methods with AMR

-- Testing performance of multidimensional, reactive numerical models

H_2-Air Mixture Ignited in a Channel with Obstacles

Beginning of Movie:

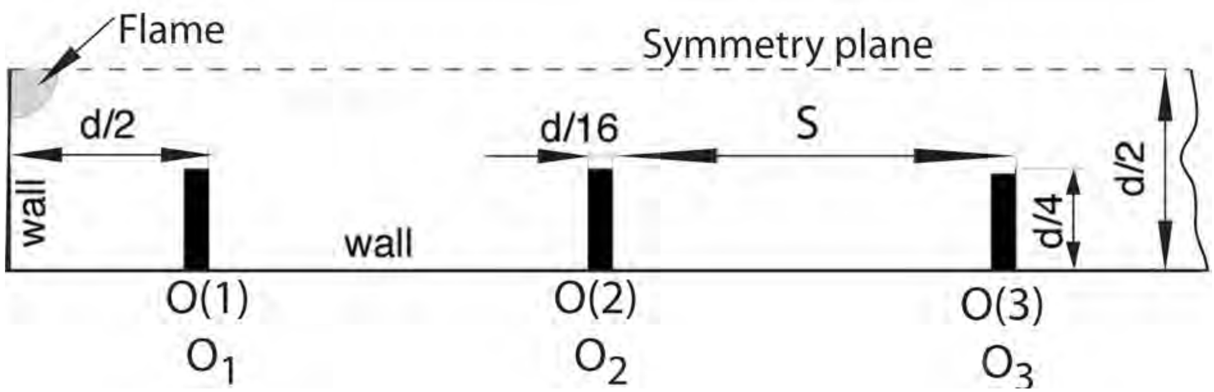


Movie will show how ...

... 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.

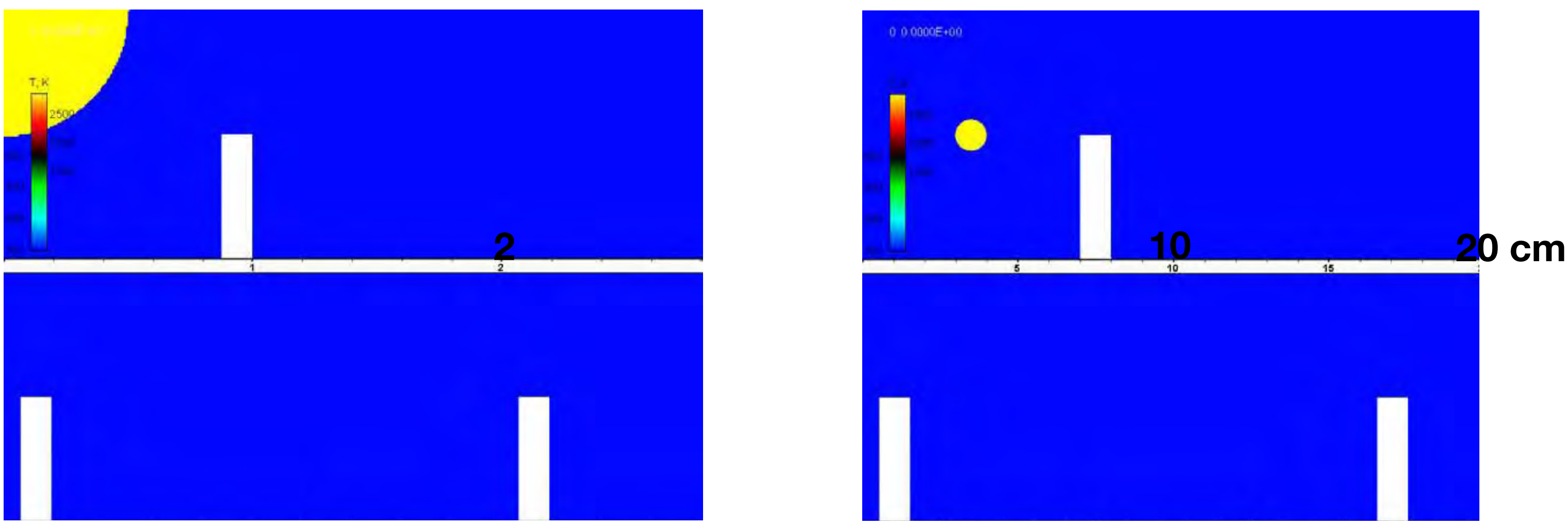
Channels with Obstacles

Channels filled with stoichiometric H_2-Air



d/2 = 1, 2, 4, **or** 8 **cm**; **Constant blockage ratio**

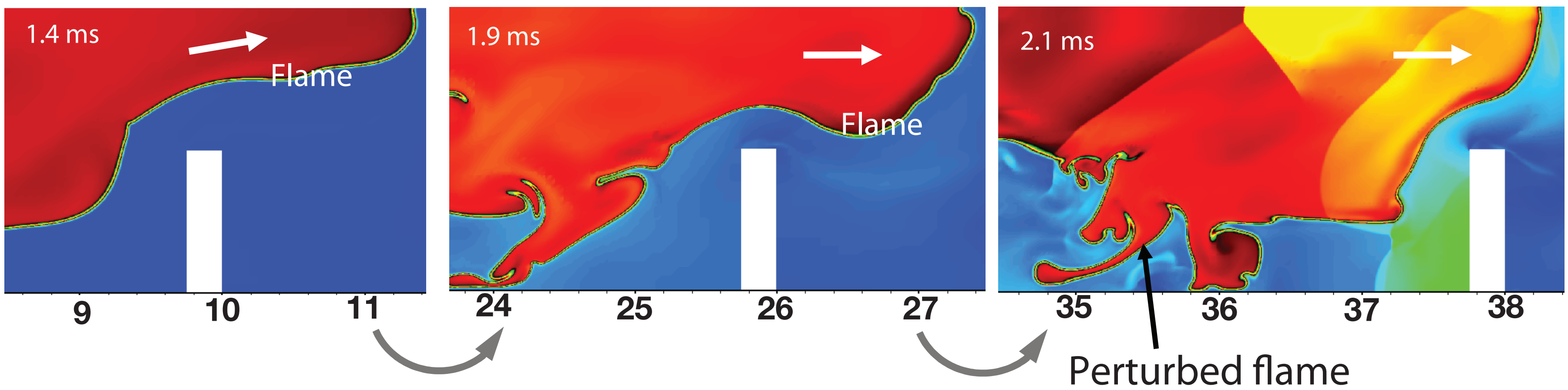
Smooth or spark ignition; Constant input energy



Computational Result

Early Flame Propagation

Temperature Contours

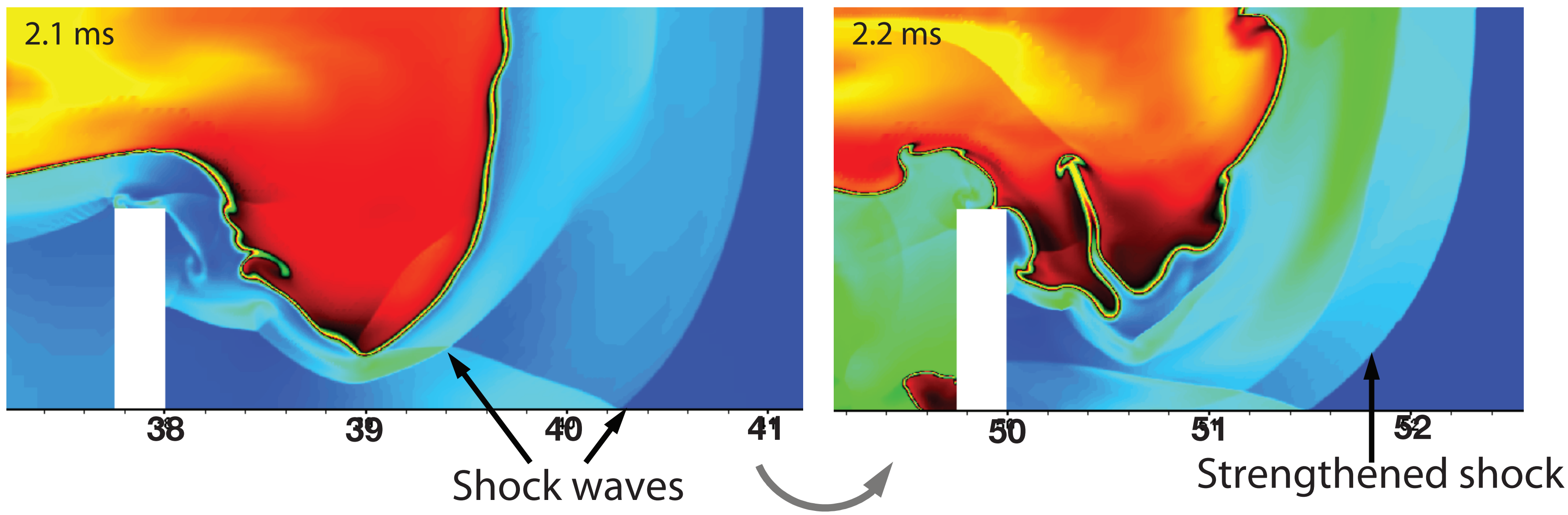


- **The initially laminar flame moves slowly into the unreacted material (to the right).**

- **Obstacles perturb the flow, which then interacts with and distort the flame, so that the flame becomes turbulent.**

Computational Result
Shock Wave Formation

Temperature Contours

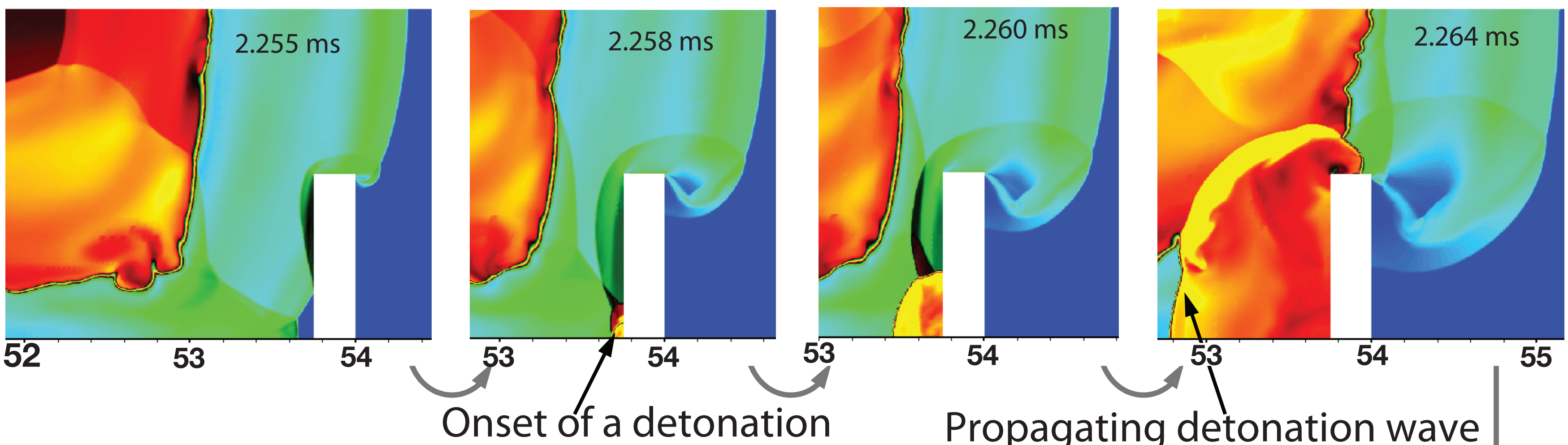


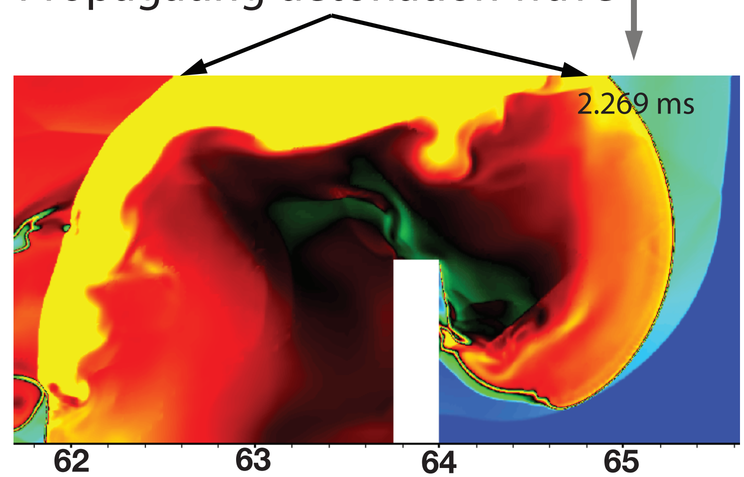
- **The turbulent flame generates compression waves, which eventually coalesce to form a shock in front of the flame.**
- **The shock is continuously strengthened by compression waves coming from behind.**

Computational Result

Transition to Detonation

Temperature Contours

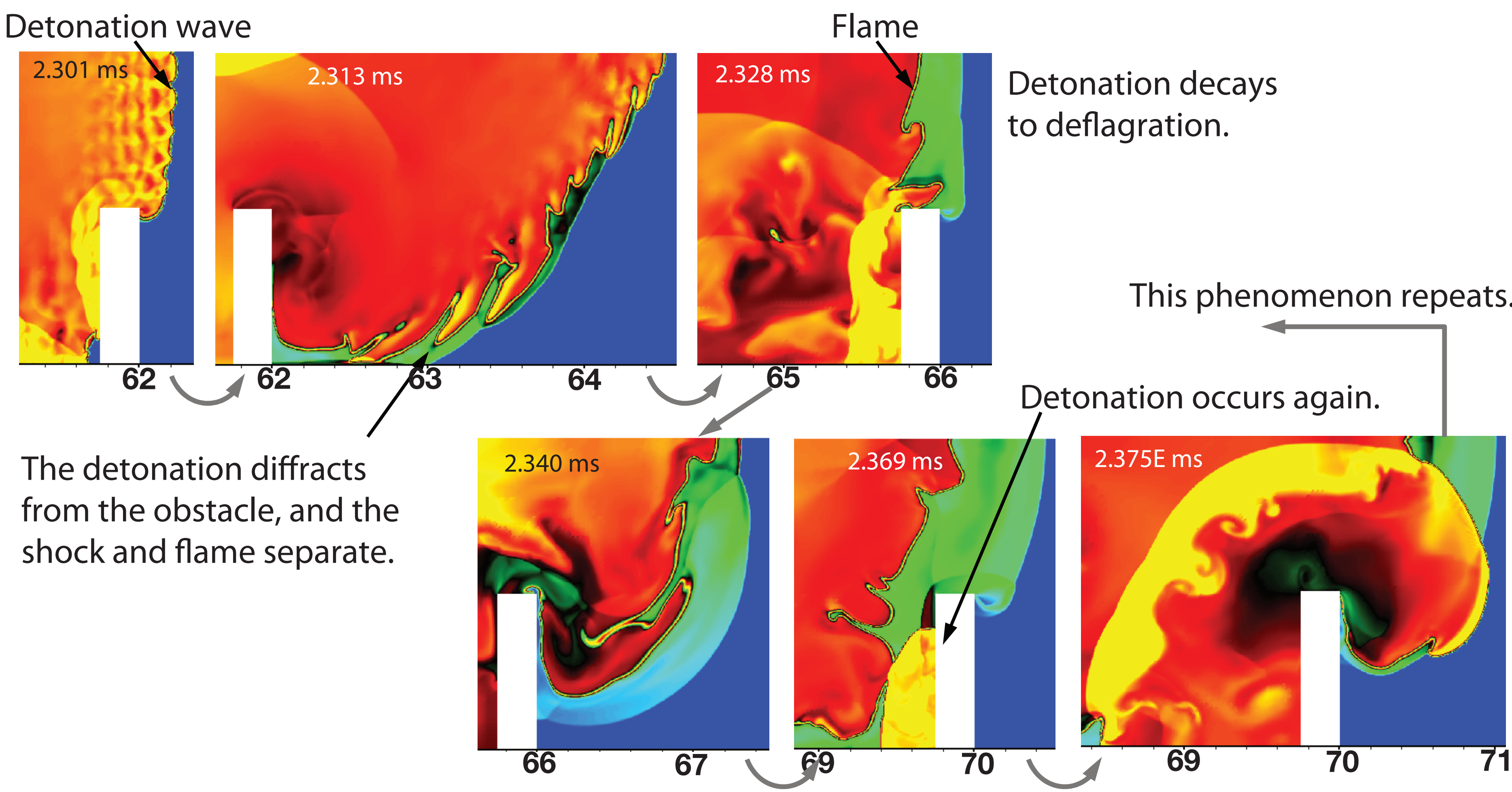




- **The shock reflects from an obstacle ... creates a hot spot ... which becomes a spontaneous wave ...**
- **A detonation wave results that *may or may not* survive.**

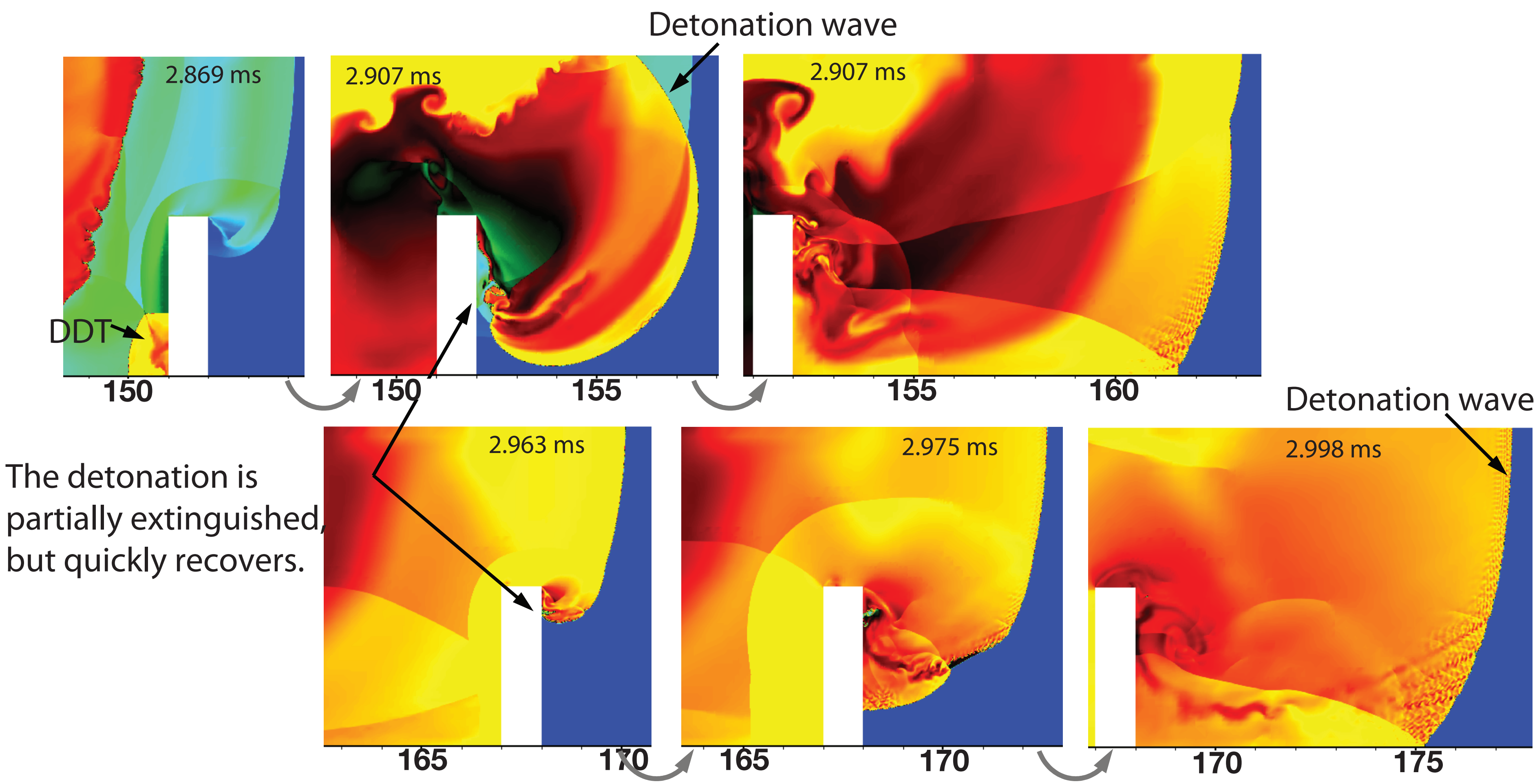
Computational Result
Detonation Wave Propagation

Quasi-detonation for d = 4 and 8 cm

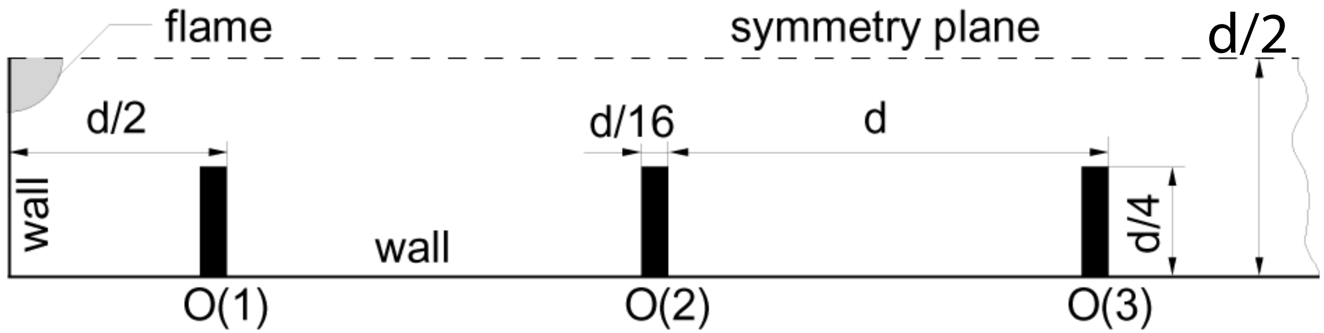


Computational Result
Detonation Wave Propagation

For large enough channels, the detonation successfully propagates over the obstacle.



Regimes of Flame Propagation



1. Slow deflagrations **subsonic**

2. Fast deflagrations ("choking") **1/3 - 1/2 D_{CJ} ,**
$\leq c_s$ in burned gas

Flame decoupled from leading shock, spreads through molecular or turbulent diffusion and convection.

3. Quasi-detonations **$< D_{CJ}$**

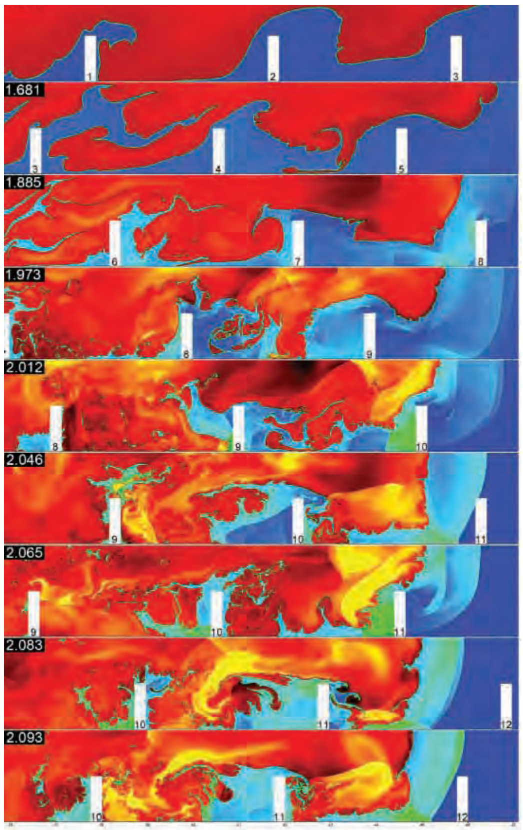
Shock & flame coupled some sometimes when reaction triggered by shock compression. Sometimes, shock and flame decoupled as detonation defracts over obstacles. Observed when width of unobstructed part of channel > few times l. Propagation velocity increases with d/l, and reachds D_{CJ} when propgation becomes indepenent of diffraction effects.

4. Detonations **D_{CJ}**

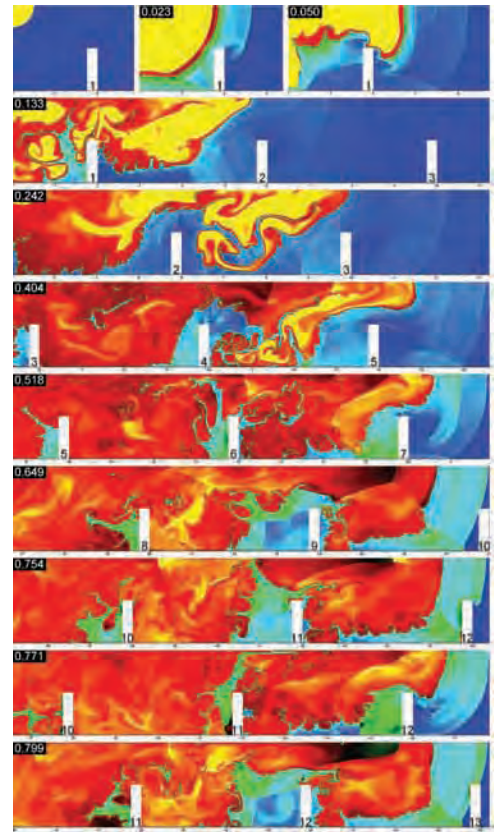
H_2-Air Mixture Ignited in a Channel with Obstacles

Two Modes of Ignition

Smooth Flame Ignition



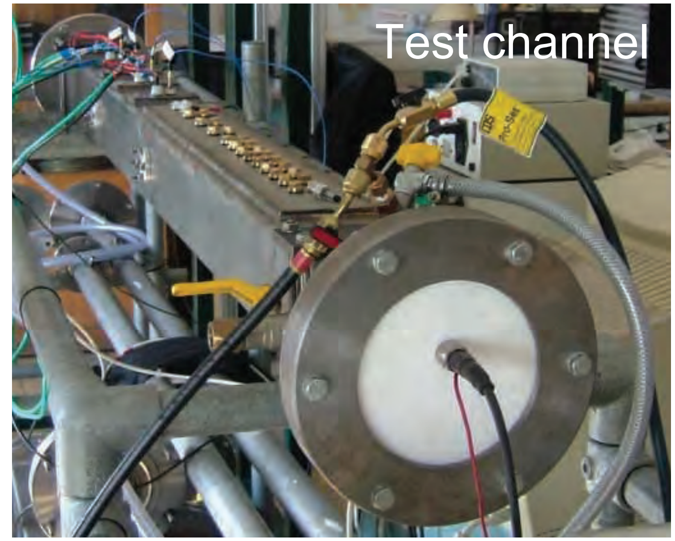
Spark Ignition

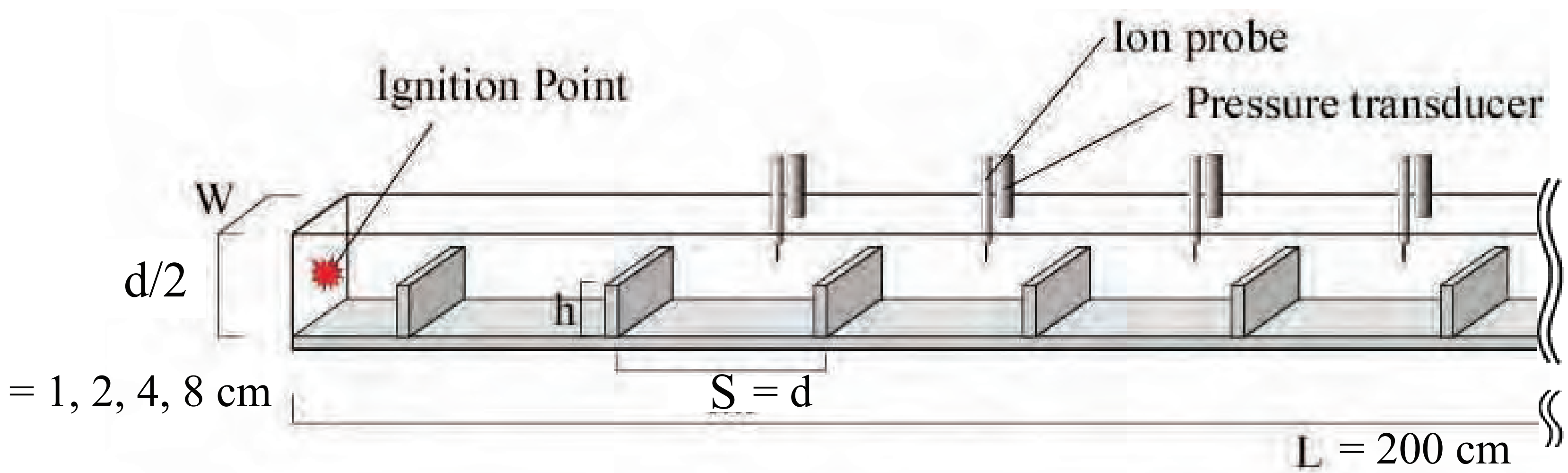


Initial development apears quite different: Immediate effects of shocks apparent for spark ignition.
Time to DDT less for spark ignition (0.61 ms from 0.76 ms)
Location is essentially the same.

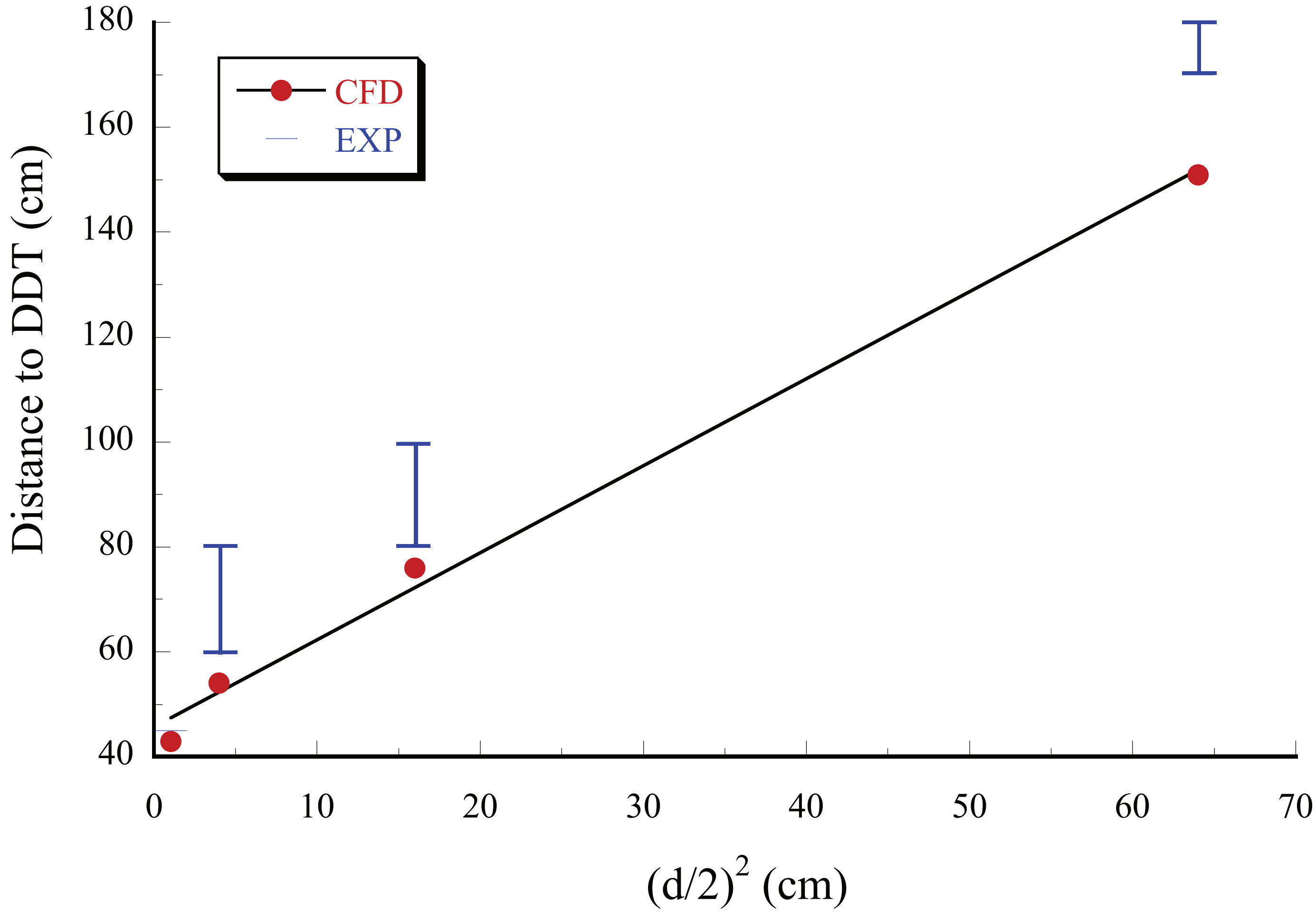
Experimental Tests

- **DDT in a channel with obstacles**
  - **For example, piping space**
  - **The same conditions as computations**
- **Conducted by Andrej Teodorczyk Warsaw University of Technology**



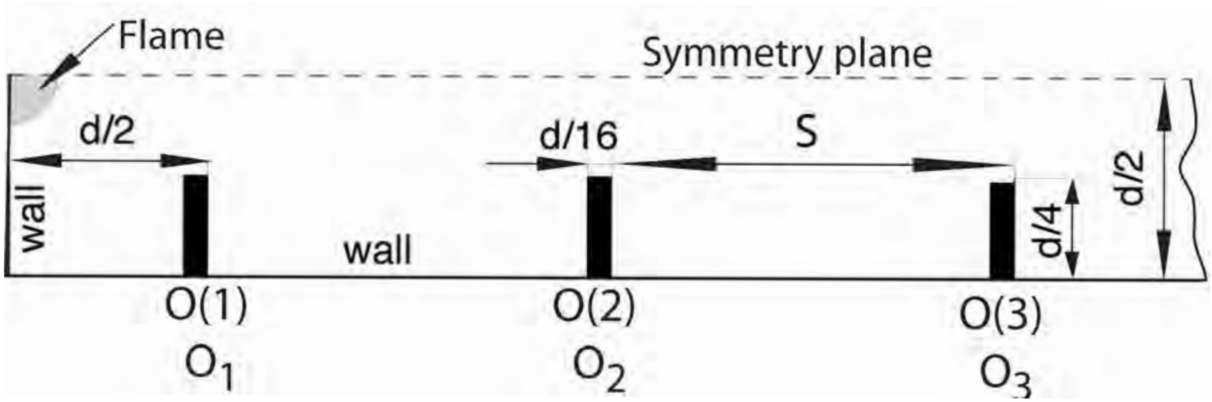


Effect of Channel Height on DDT Distance



The distance to DDT is proportional to d^2

Cases Considered for H_2-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 compex geometries

Why do simulations "work" ..?

Effects of non-Kolmogorov turbulence

Stochasticity

THE PHYSICAL MODEL

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

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

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

$$\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho Y \mathbf{U}) + \nabla \cdot (\rho D \nabla Y) - \rho \dot{w} = 0 \,,$$

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

$$P = \frac{\rho R T}{M} \,, \qquad E = \frac{P}{(\gamma - 1)} + \frac{\rho U^2}{2} \,,$$

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

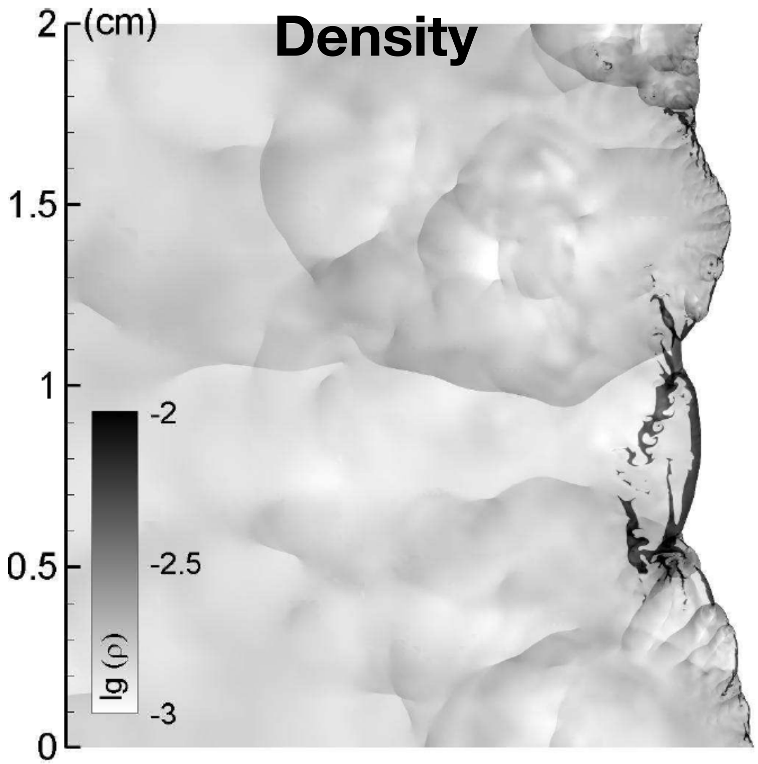
$$\nu = \nu_0 \frac{T^n}{\rho} \,, \quad D = D_0 \frac{T^n}{\rho} \,, \quad \frac{K}{\rho C_p} = \kappa_0 \frac{T^n}{\rho}$$

$$Le = \frac{K}{\rho C_p D} = \frac{\kappa_0}{D_0} \,, \quad Pr = \frac{\rho C_p \nu}{K} = \frac{\nu_0}{\kappa_0} \,, \quad Sc = \frac{\nu}{D} = \frac{\nu_0}{D_0}$$

Material, Chemistry, and Reaction Wave Parameters
Stoichiometric Hydrogen-Air

Quantity	Value	Definition
Input		
T_0	293 K	Initial temperature
P_0	1 atm	Initial pressure
ρ_0	8.7345×10^{-4} g/cm^3	Initial density
γ	1.17	Adiabatic index
M	21 g/mol	Molecular weight
A	6.85×10^{12} cm^3/g-s	Pre-exponential factor
$E_a (= Q)$	$46.37\, RT_0$	Activation energy
q	$43.28\, RT_0/M$	Chemical energy release
$\nu_0 = \kappa_0 = D_0$	2.9×10^{-5} g/s-cm-K$^{0.7}$	Transport constants
Output		
S_l	298 cm/s	Laminar flame speed
T_b	7.289 T_0	Post-flame temperature
ρ_b	0.1372 ρ_0	Post-flame density
x_l	0.035 cm	Laminar flame thickness
D_{CJ}	1.993×10^5 cm/s	CJ detonation velocity
P_{ZND}	31.47 P_0	Post-shock pressure
P_{CJ}	16.24 P_0	Pressure at CJ point
T_{ZND}	3.457 T_0	Post-shock temperature
T_{CJ}	9.010 T_0	Temperature at CJ point
ρ_{ZND}	9.104 ρ_0	Post-shock density
ρ_{CJ}	1.802 ρ_0	Density at CJ point
x_d	0.01927 cm	1D half-reaction thickness
λ	1–2 cm	Detonation cell size

A two-dimensional calculation of a propagating detonation, with enough resolution, produces reasonable detonation cell structure



Backgrond: 1 atm, 293 K
Stoichiometry H_2-air
Mininum dx = 1/2048 **cm**

Two-level detonation cell structure,
λ = 1 - 2 cm

Hot-Spot Ignition in Stoichiometric Hydrogen-Air

Consider three different gradients.
dx = 0.016 cm, uniform mesh.

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

C **is concentraion (mass fraction of unburned material)**

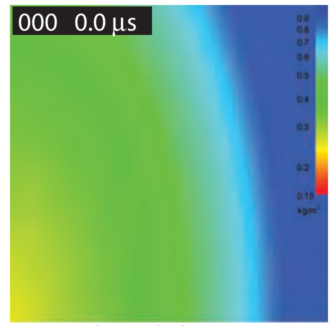
$$\frac{dC}{dx} = \frac{0.4}{R} \quad \text{and} \quad \frac{dC}{dy} = 2\,\frac{dC}{dx}$$

Result is an elliptical distribution.

At the center,

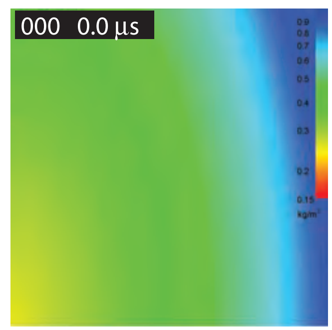
$$C = 0.6 \quad T = 1029\ K$$

8.192 cm

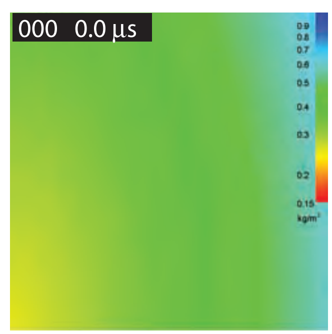


8.192 cm

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



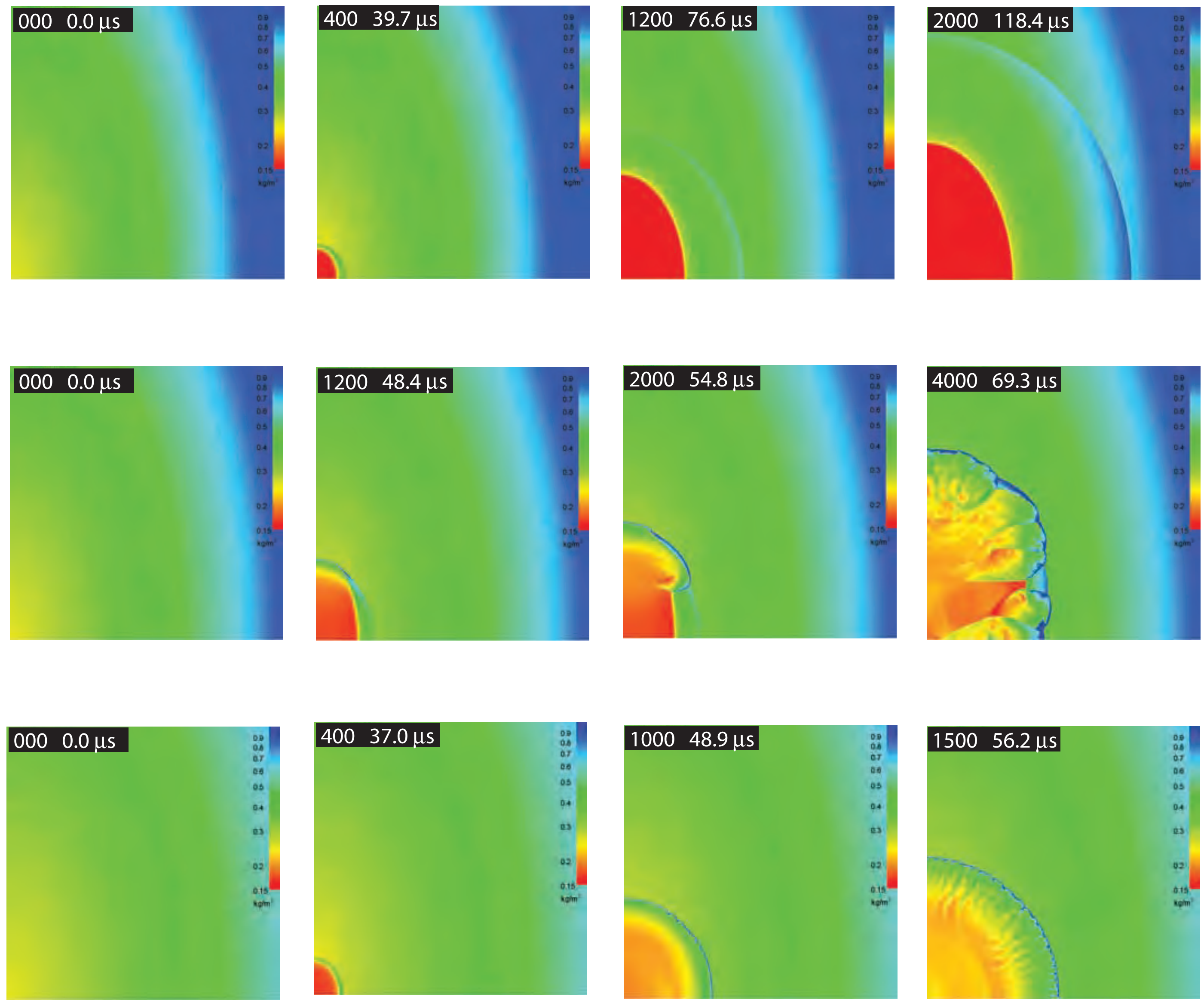
R = 10
Detonation appears in both directions

Hot-Spot Ignition in Stoichiometric Hydrogen-Air

Case 1 --
Ignition in gradient leaves a shock and a flame

Case 2 --
Ignition in gradient - intermediate case

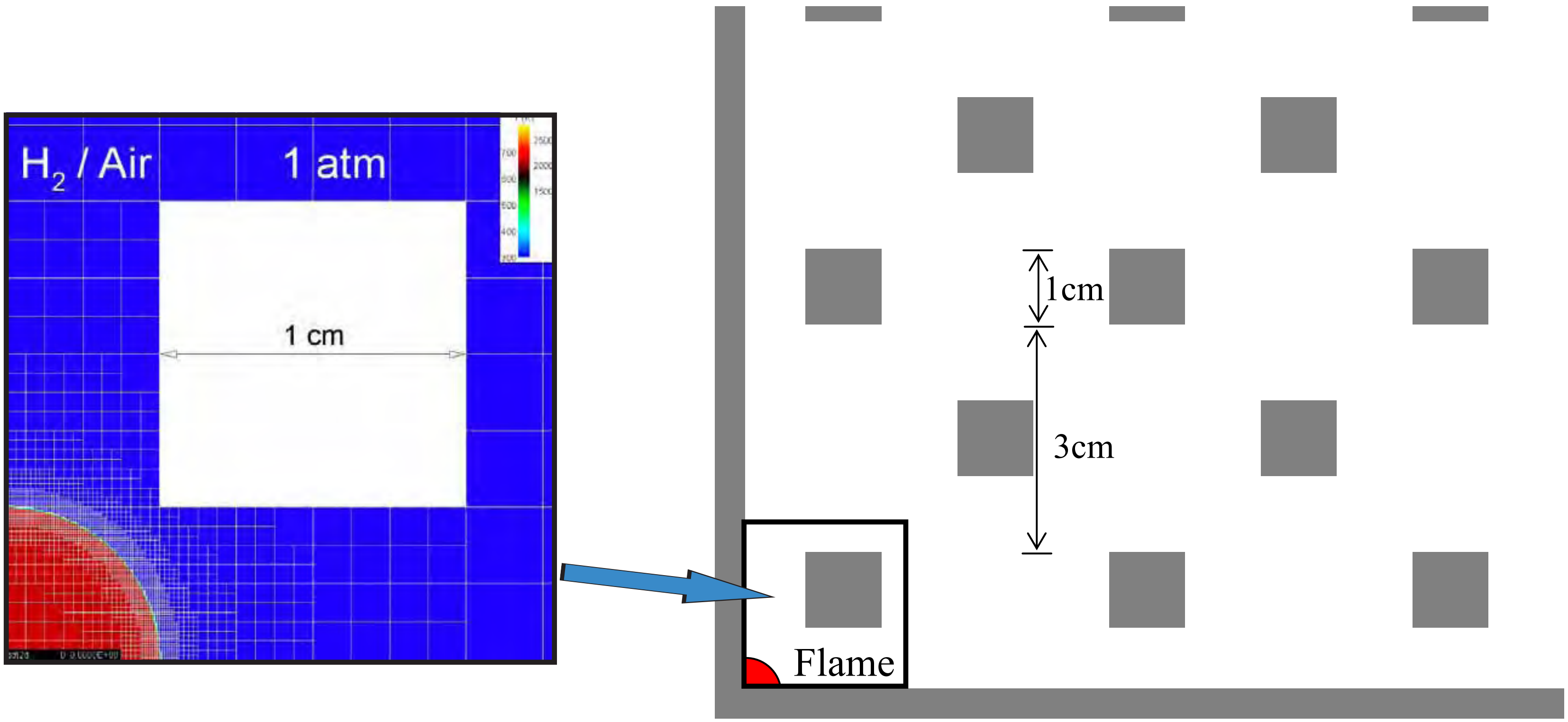
Case 3
Ignition in gradient produces a detonation



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

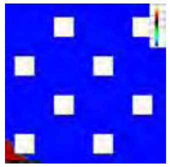
An Array of Obstacles

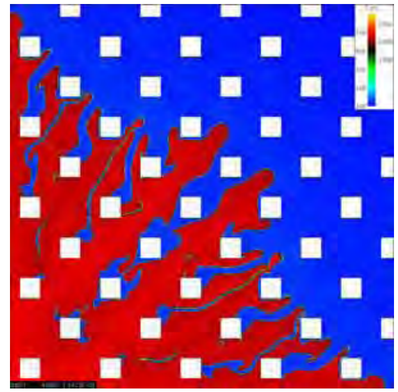
- **Array of 1 cm x 1 cm square obstacles**
- **H_2-Air background**
- **Staggered layout**



DDT in an Array of Obstacles

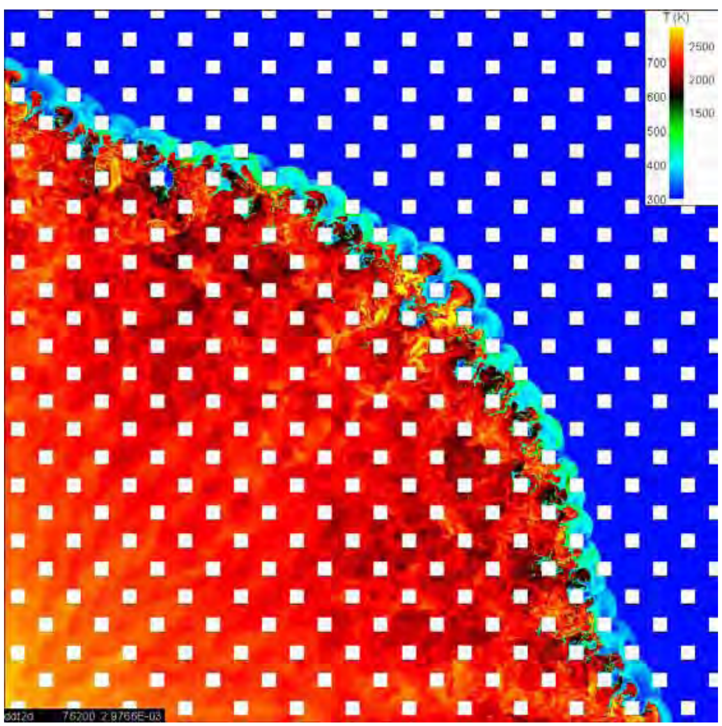
1. Initial flame



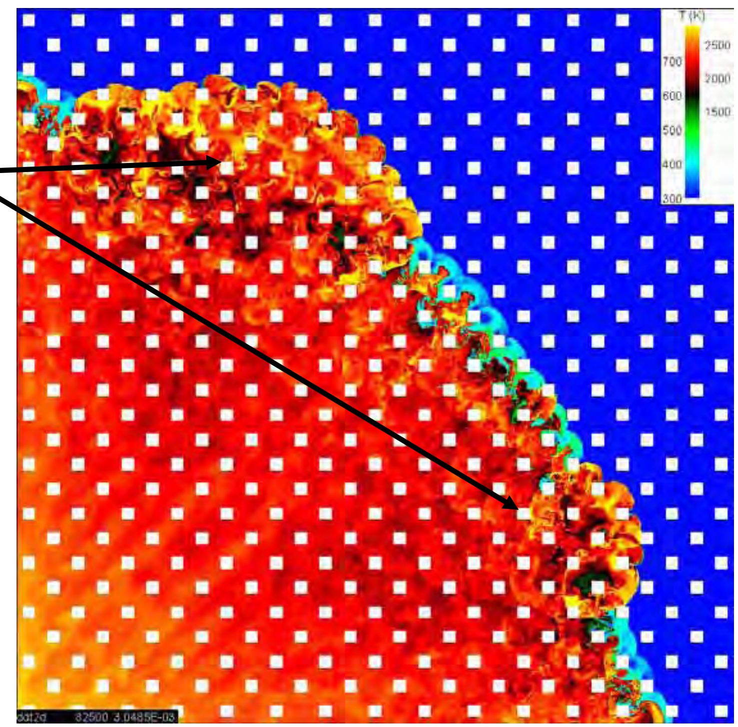


2. The flame becomes turbulent.

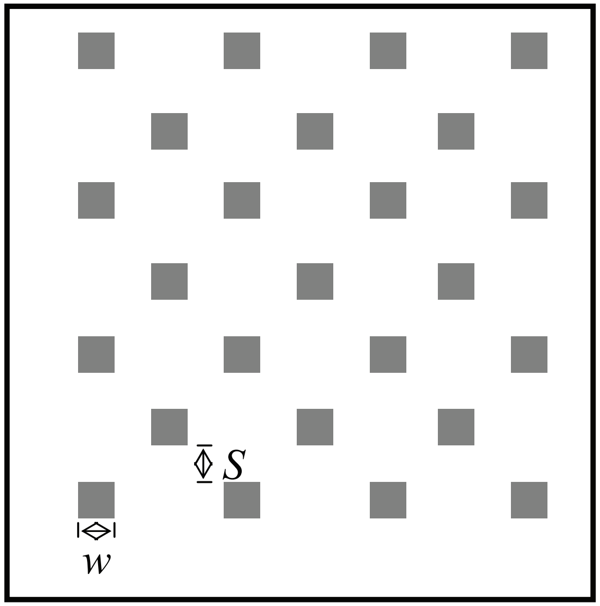
3. Shock wave formation



4. DDT: shock reflection from obstacles

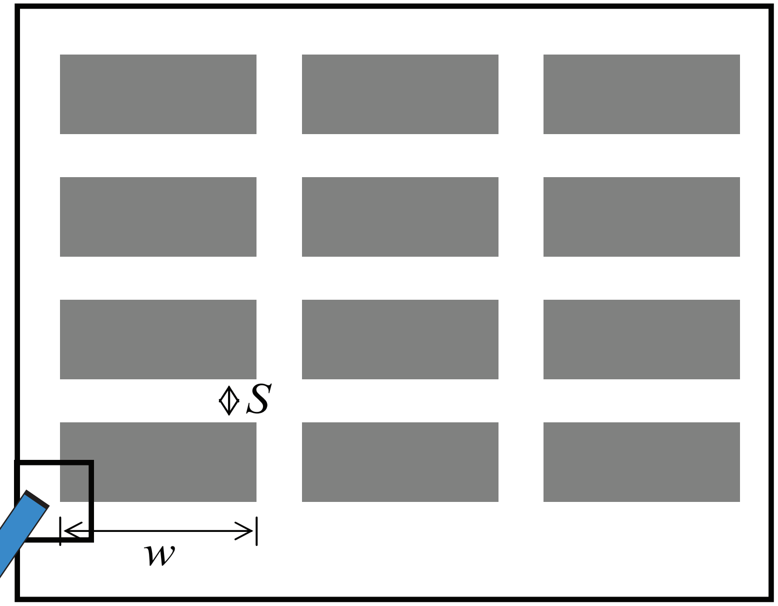


Array of Obstacles

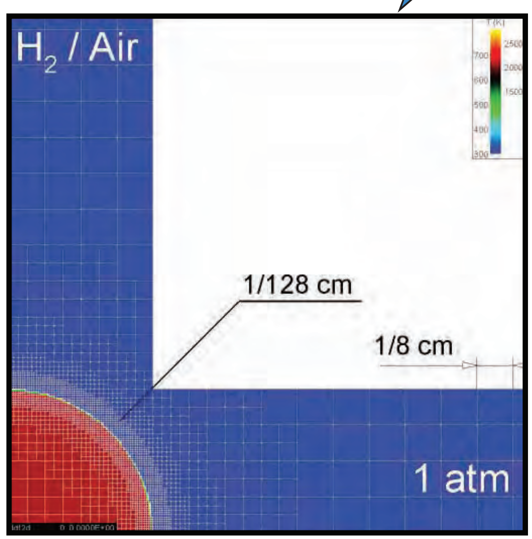


$S = 1$ cm, $w = 1$ cm
(staggered)

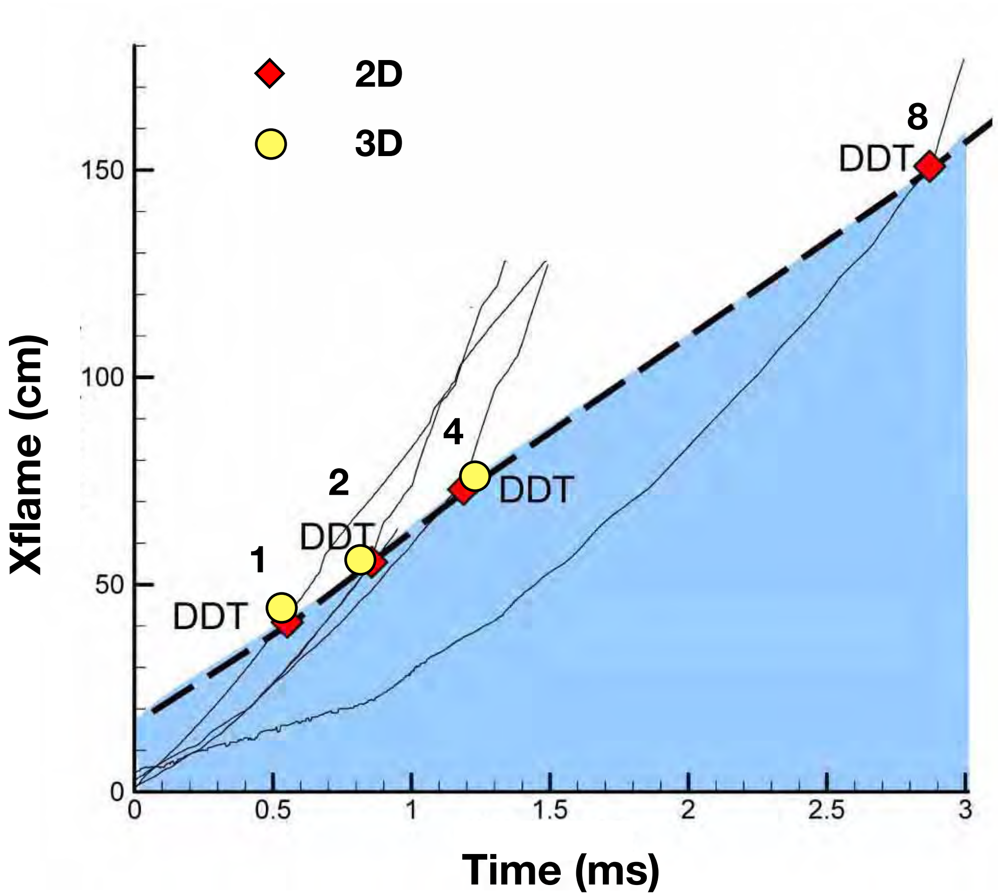
Different size and layout



$S = 1$ cm, $w = 4$ cm
(symmetric)



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



DDT = First successful hot-spot transition

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

Two Effects to Note:
- **Ignition of Hot Spots**
- **Effect of Scale**
  - **System has to be big enough to sustain DDT**

These are related ...

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 simultaneouly.

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