The Laminar-to-Turbulent-Detonation Transition: Hot Spots, Turbulence, and Stochasticity

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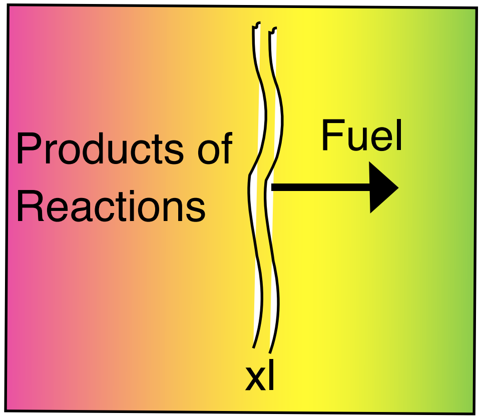
Some Background Terminology ...

Laminar Flame

M << 1

Energy Release
Expansion
Thermal Conduction
Molecular Diffusion
Radiation ....



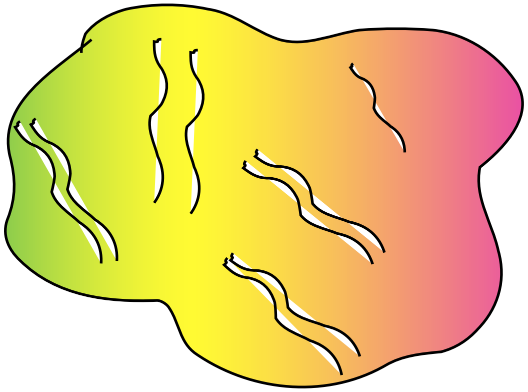
Products of Reactions

Fuel

xl

Turbulent Flame

M < 1



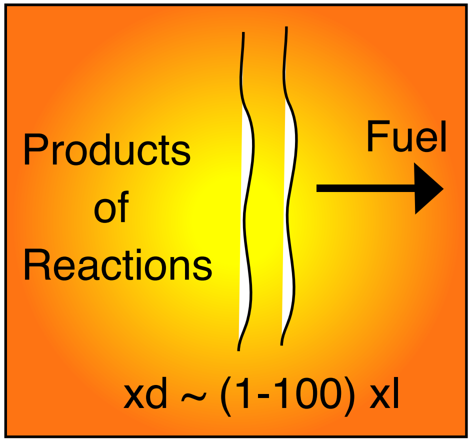
Wide Range of Conditions:
- Flamlets
- Distributed Flames
- Shocks ...

Deflagration ...
"Vigorous burning with subsonic flame propagation"

Detonation

M > 1

Energy Release
Compressible Flow
Shocks, and
Complex Shock Structures ...



Products of Reactions

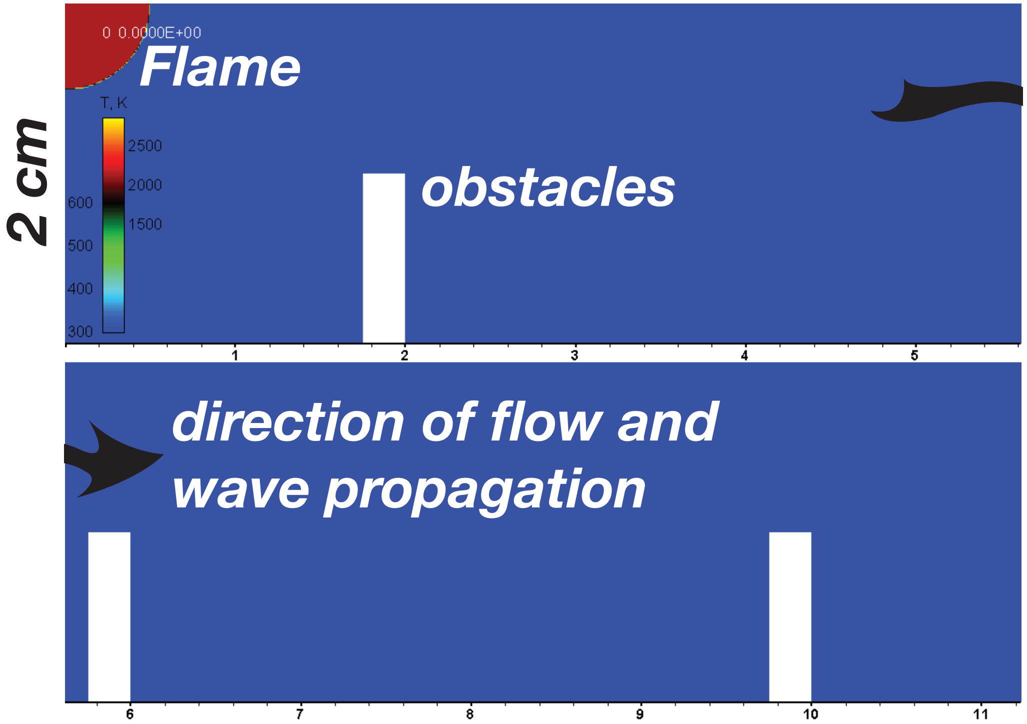
Fuel

xd ~ (1-100) xl

Transitions among these states are not as well understood.

H_2-Air Mixture Ignited in a Channel with Obstacles

Beginning of Movie:



Movie will show how ...

Starting with a small flame in a channel containing a combustible mixture, a turbulent flames develops and produces shock waves.

This leads to the formation of unsteady shock-flame complexes and detonations.

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
	$E_a (= Q)$	$46.37\, R T_0$	Activation energy
	q	$43.28\, R T_0 / M$	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

Solution Approach

Solve the unsteady, compressible Navier-Stokes equations in one-, two-, and and three-dimensions by (at least) two different numerical methods: a lower-order Gudonov method (Gamezo) and a high-order FCT method (Ogawa).

Include (calibrated) models for chemical reactions, energy release, thermal conduction, and molecular diffusion.

Resolve the flow down to viscous microscale (if needed), using adaptive mesh refinement (AMR) based on the fully threaded tree (FTT) algorithm for mesh refinement.

Simulate specific laboratory experiments, some specifically designed to test the model

E.g., Studies of DDT (Thomas et al.)
Flame acceleration (Teordorczyk et al.)
Natural gas (Kuznetzov et al., Zipf et al.)

Can we reproduce phenomena observed and measured?

A range of geometries, initial conditions, and reactive materials have been studied ...

Material: Ethylene and acetylene (low pressure)
Thermonuclear C-O system (white dwarf star)
Hydrogen (atmospheric; stoichiometric)
Methane (atmospheric; stoichiometric, lean)

Dimension: 1, 2, and 3 dimensions

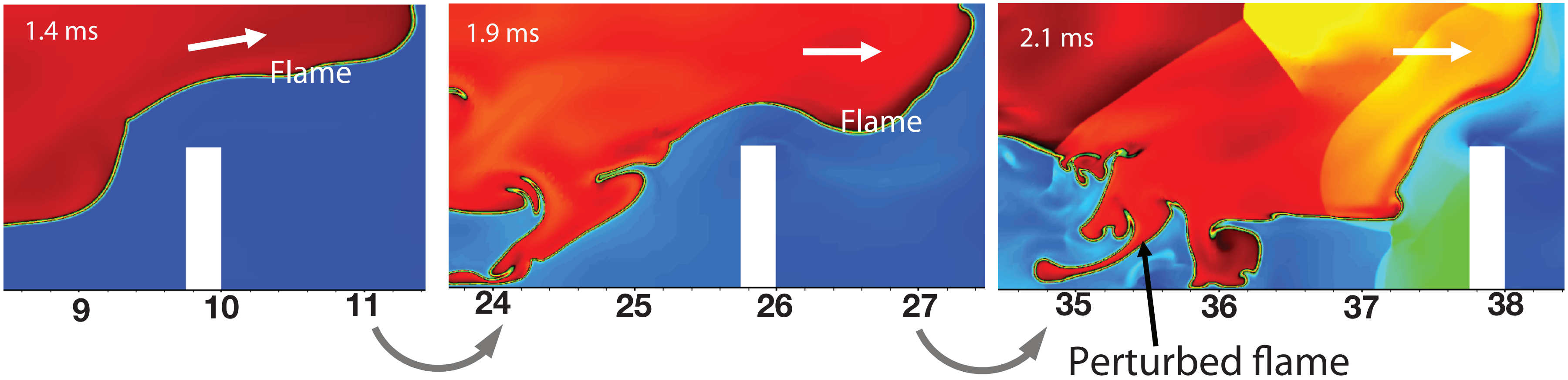
Geometrical Configurations:
Channels and chambers. Vary: size; blockage ratio; boundaries; obstacle geometry, spacing, symmetry
Open: Spherical (white dwarf), level of turbulence

Mode of ignition: Shock-flame interactions
Smooth or spark

... etc.

Early Flame Propagation

Temperature Contours



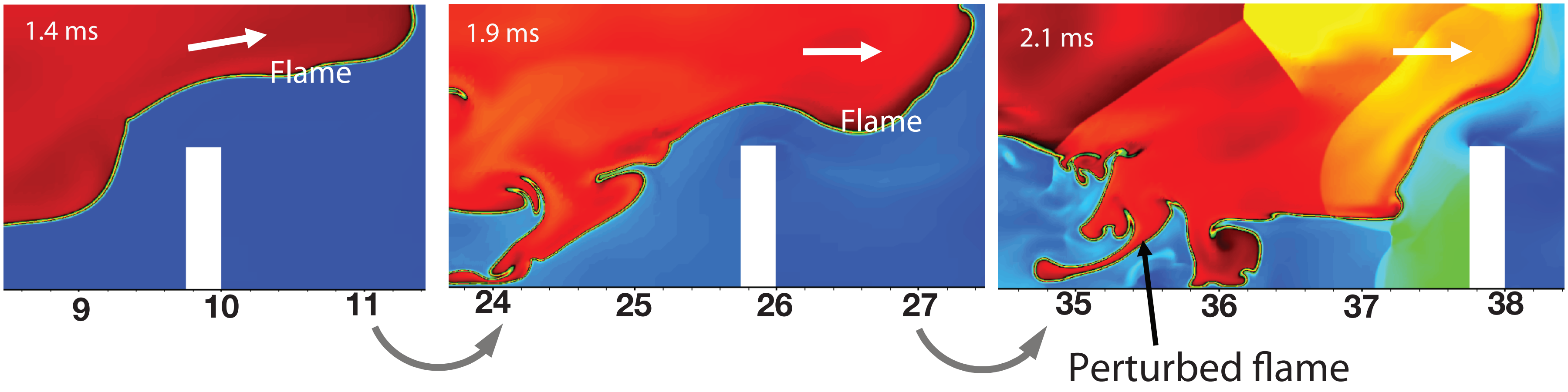
- **The initially laminar flame moves slowly into the unreacted material (to the right).**

This is when fluid-diffusive-chemical instabilities may become important. They can wrinkle the flame front and so increase the energy-release rate.

On the time scales of this simulation, these instabilities might not have a major effect on the dyamics before other, stronger interactions come into play.

Early Flame Propagation

Temperature Contours



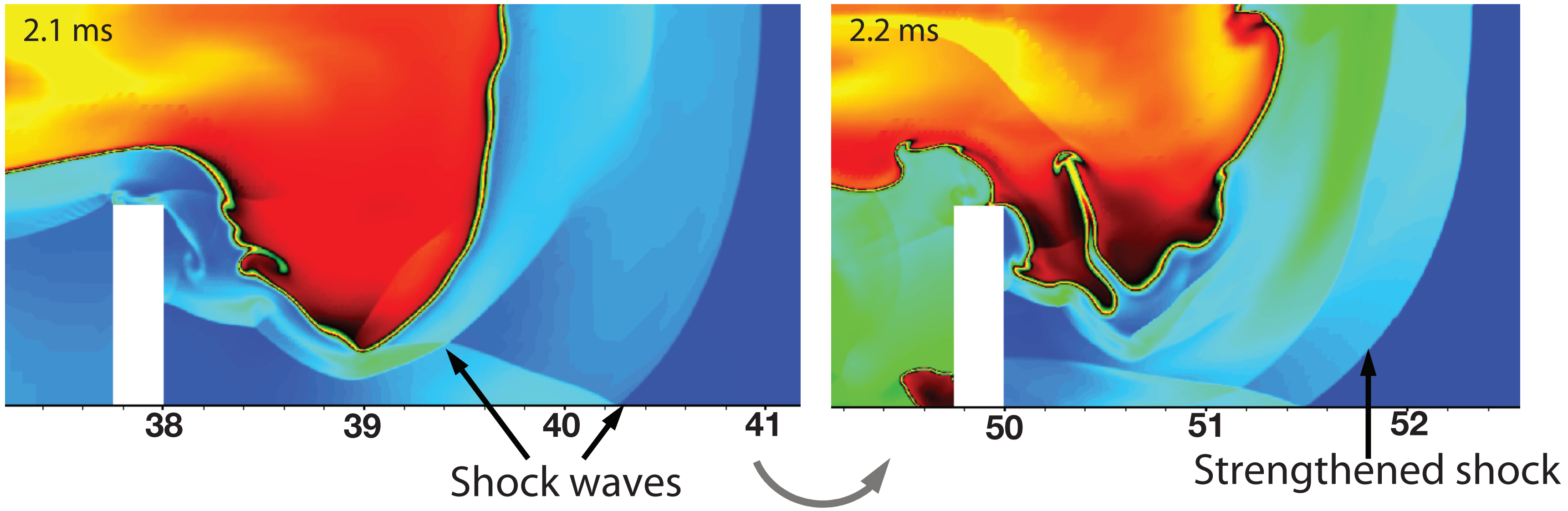
- The initially laminar flame moves slowly into the unreacted material (to the right).

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

Flow interactions with obstacles create perturbations that distort the flame. These increase the surface area of the flame, enhance energy the energy-release rate, and thus acceleratethe flame and background flow.

Shock Wave Formation

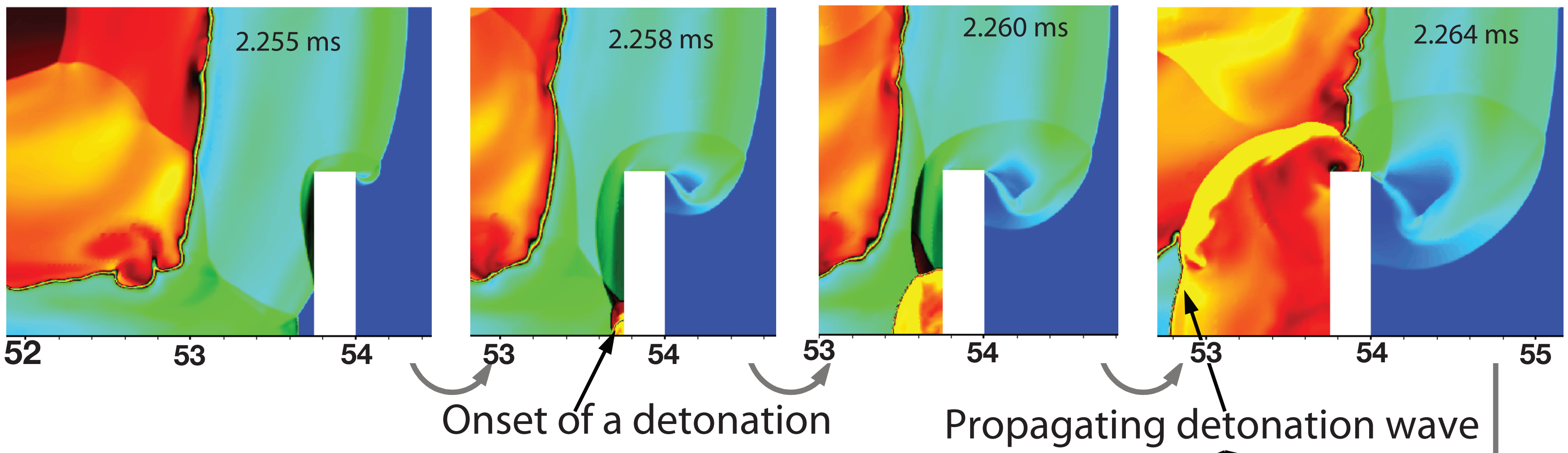
Temperature Contours



- **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.**
- **Shock-flame interactions are important - increase flame area and generate vorticity.**

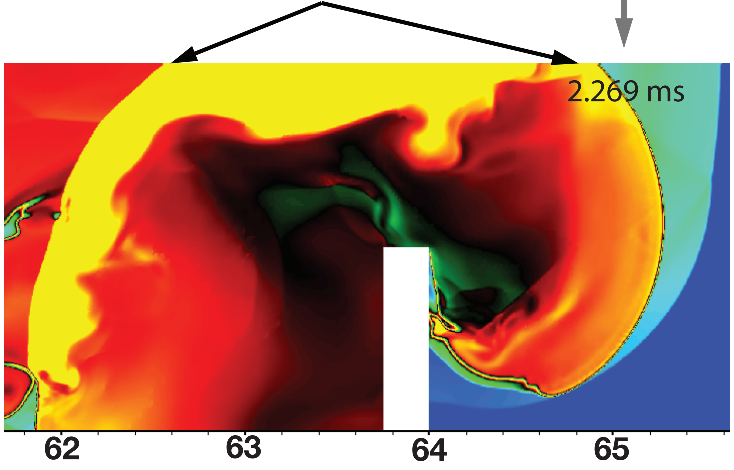
Transition to Detonation

Temperature Contours



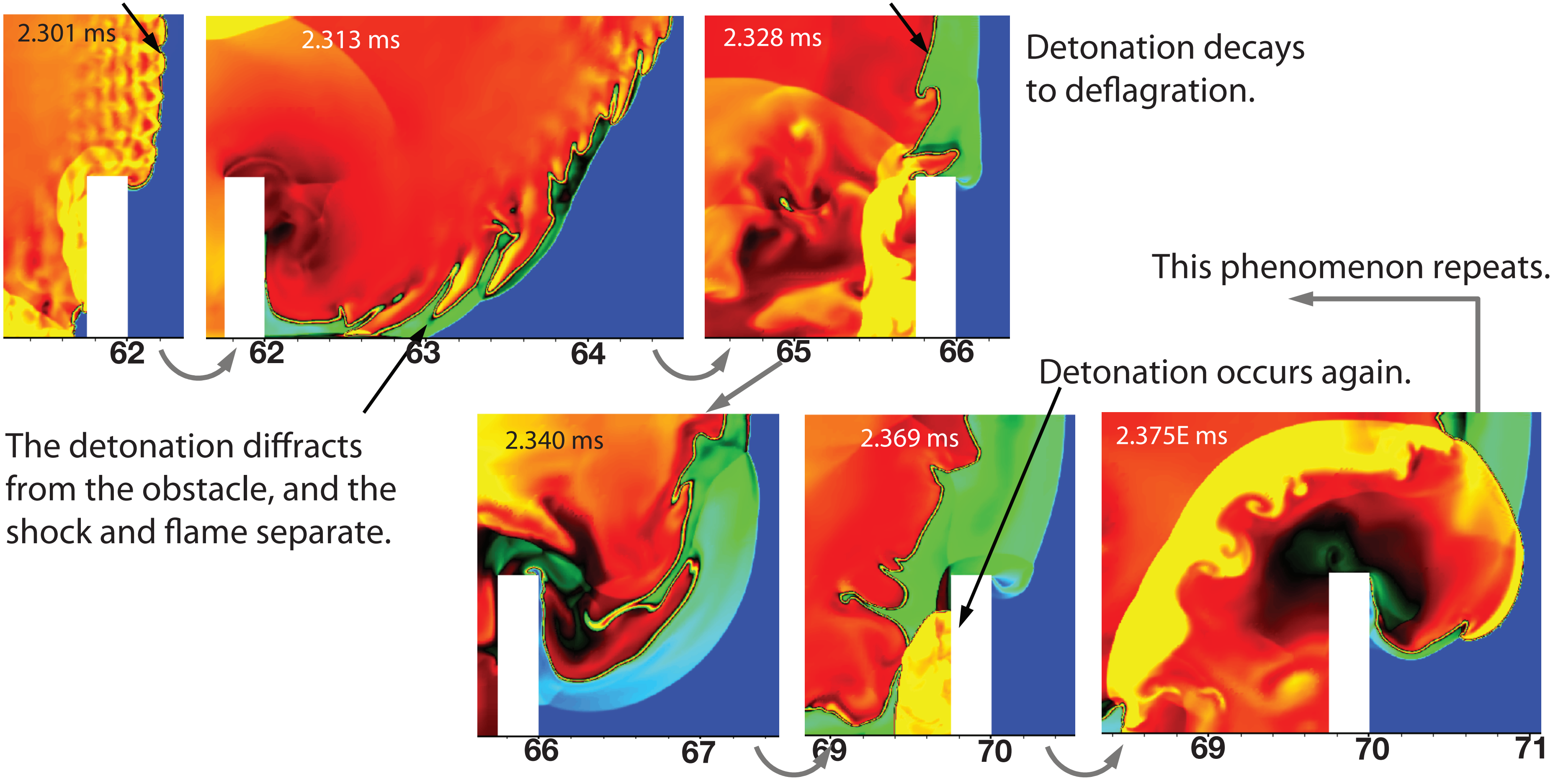
Onset of a detonation

Propagating detonation wave



- **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.**

Detonation Wave Propagation



Detonation wave

Flame

Detonation decays to deflagration.

This phenomenon repeats.

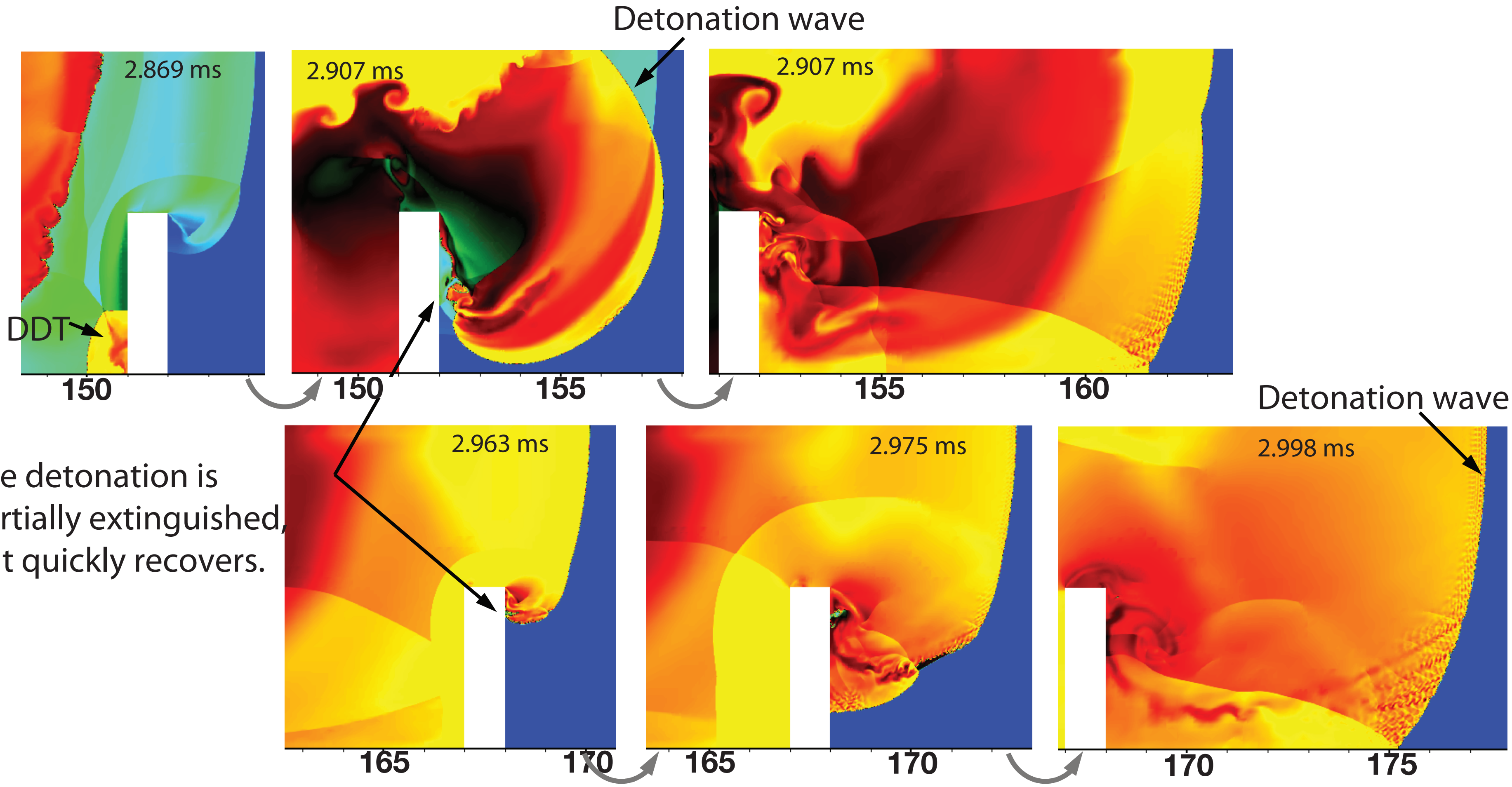
Detonation occurs again.

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

Quasi-detonation for smaller channels

Detonation Wave Propagation

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



Detonation wave

Detonation wave

The detonation is partially extinguished, but quickly recovers.

Hot Spots, Turbulence, and Stochasticity

“The turbulent flame creates the environment in the unreacted background gases in which a detonation may occur ... ”

Hot Spots

- Appear where there is unreacted material
- Start as gradients of reactivity
- Are created by inhomogeneities in the background flow (turbulence, vorticity, contact surfaces, shocks .....)
- May undergo transition to a detonation, or decay to a shock and a flame

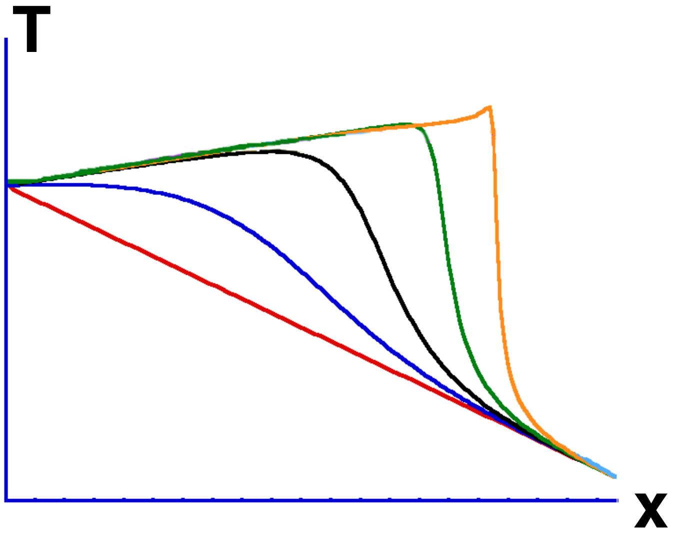
Hot Spot Physics

A hot spot is a small region in unreacted fuel in which the properties (e.g., temperature, composition, etc.) vary, so that chemical reactions can proceed faster inside the spot.

A hot spot can auto-ignite, and then give rise to a detonation, a separated shock and a flame, or just a flame.

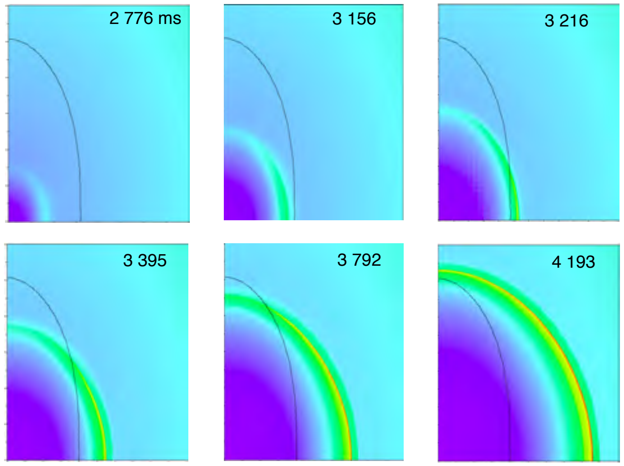
Transition to a detonation occurs by the (Zeldovich et al.) gradient mechanism: a gradient of induction time, τ_{ind}, leads to a supersonic spontaneous wave that may become a detonation.

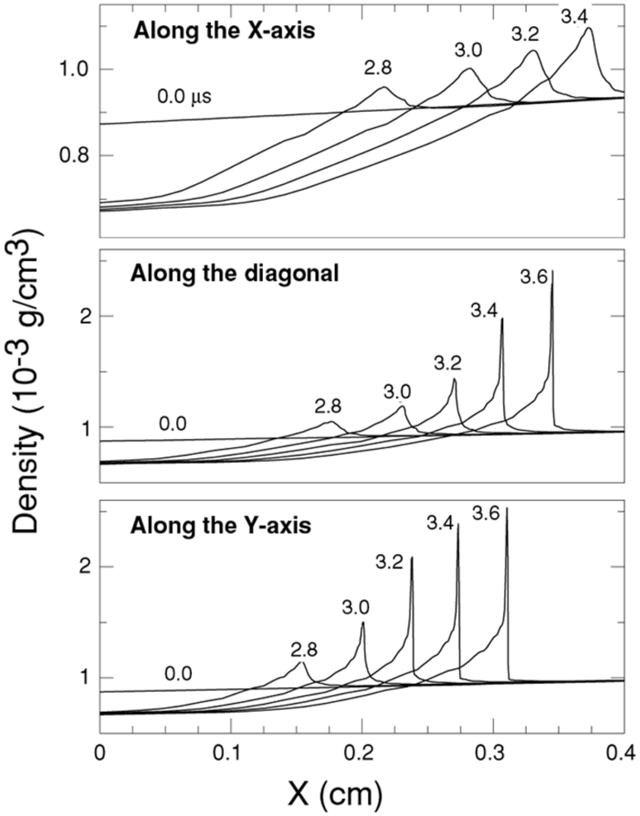
$$D_{sp} = \left(\frac{\partial \tau_{ind}}{\partial T} \right)^{-1} \frac{1}{|\nabla T|}$$

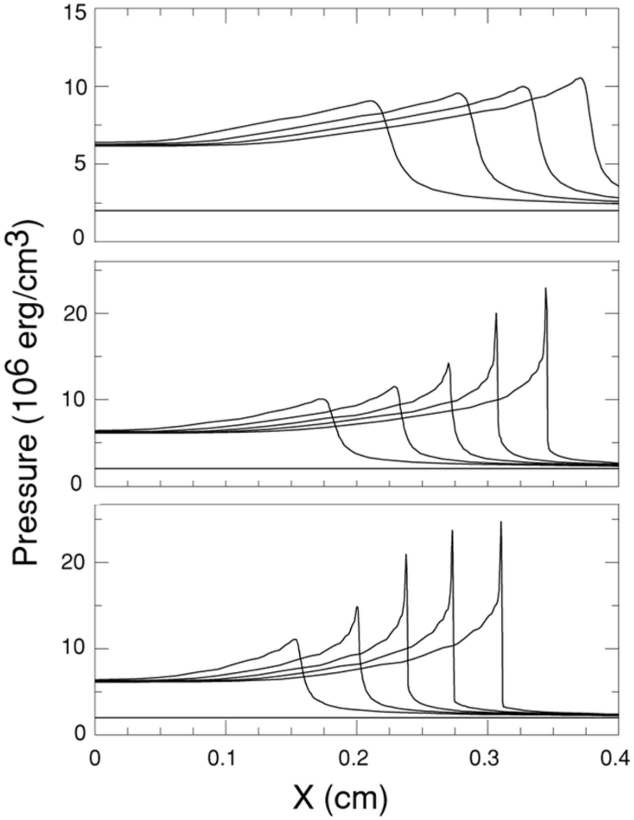


Reaction front moves spontaneously due to nonuniformity of initial distribution of temperature, composition, etc.

Evolution of the Hot Spot



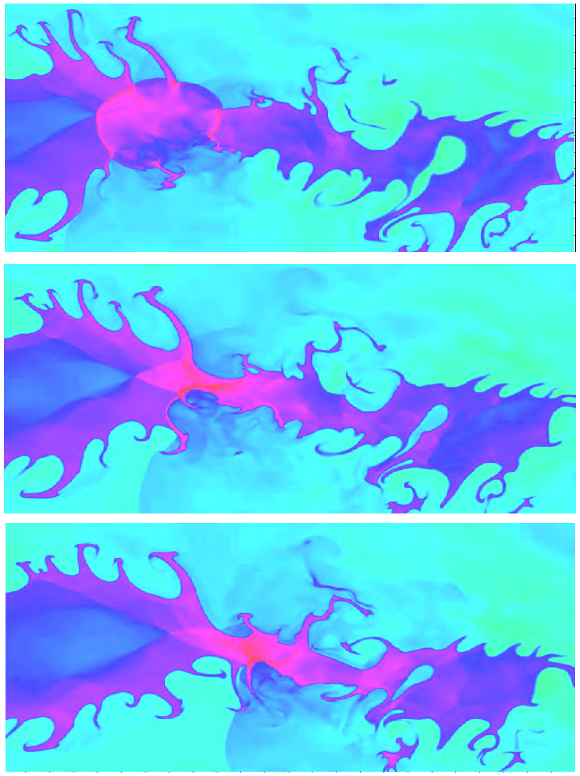




Hot Spot Physics

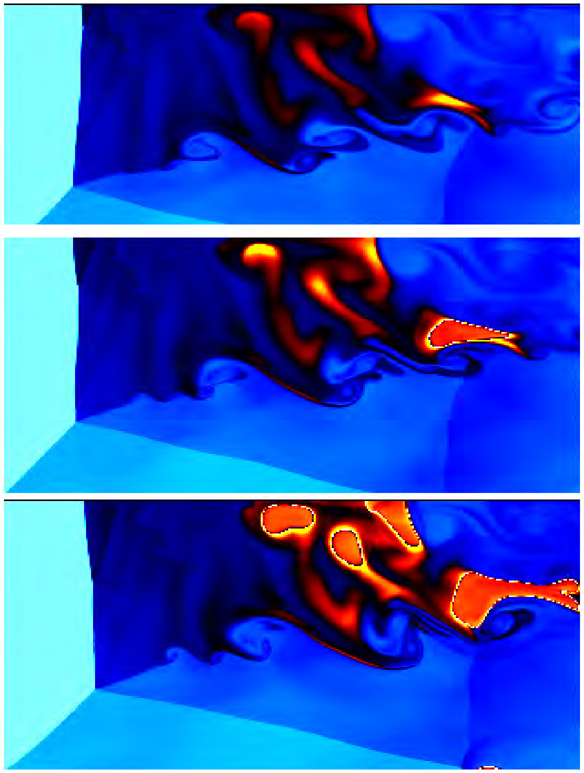
But the local environment of hot spots can be very dynamic and therefore very complex ...

Density



Acetylene-air

Temperature

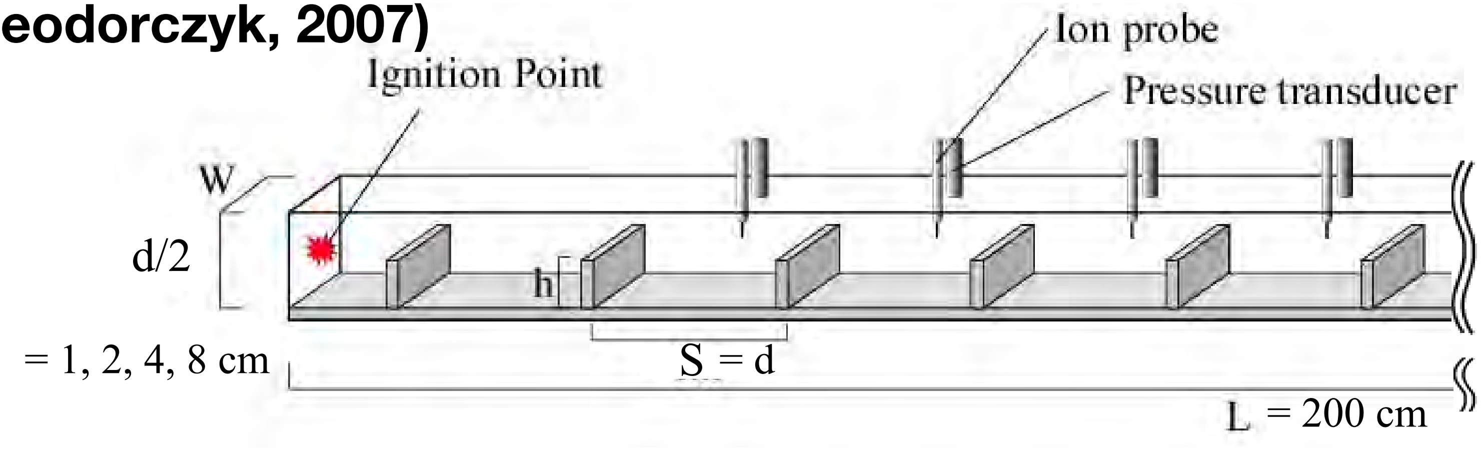


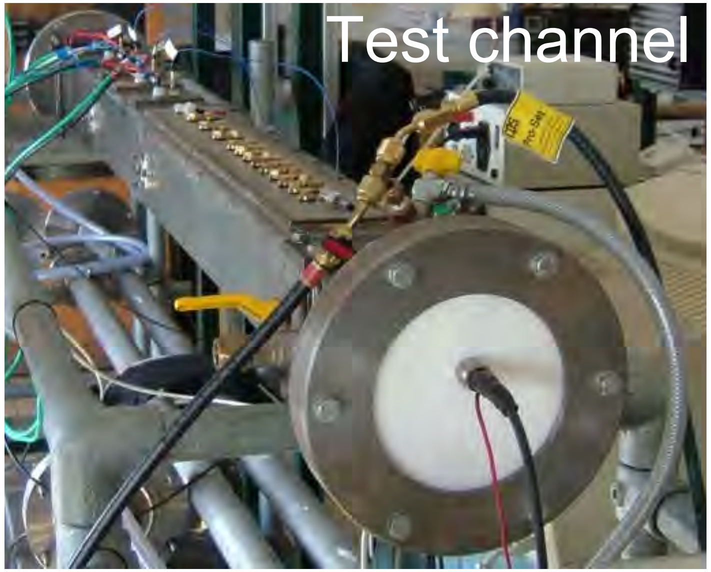
Ethylene-air

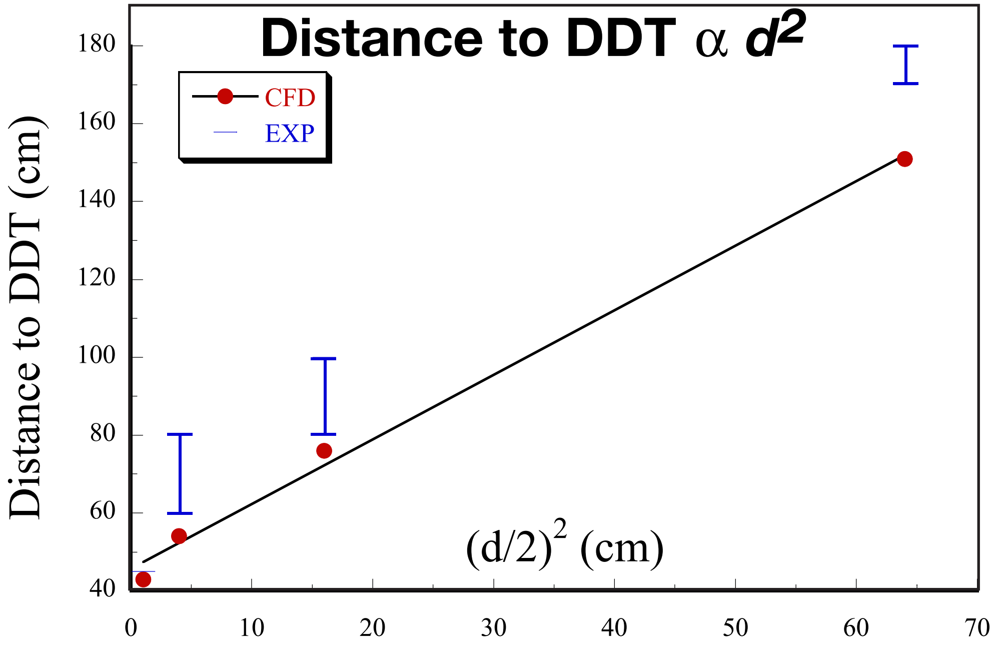
Experimental Tests

Effect of Channel Height on DDT Distance

(Teodorczyk, 2007)







What does this mean?
Why is there “good agreement” ?

2D agrees with 3D agrees with experiments?

How can this happen when the system is turbulent, chemically reacting, full of boundary layers, etc etc?

(What is this nonsense?)

A Possible Explanation

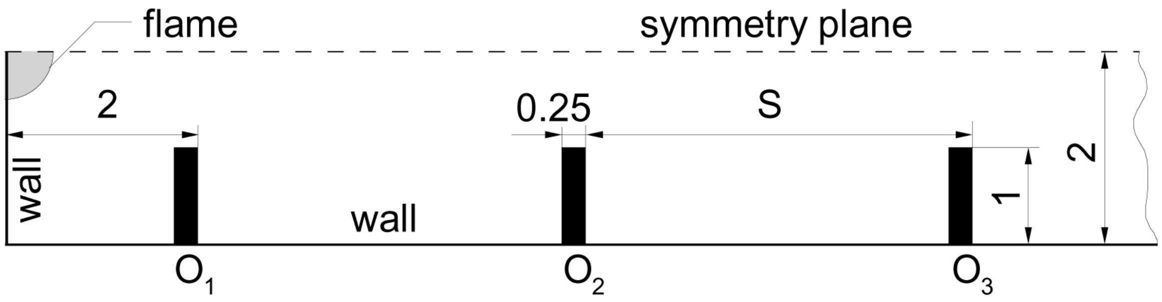
Shock-flame interactions are a major source of turbulence (vorticity generation) and flame distortion in compressible, high-speed, reactive flows.

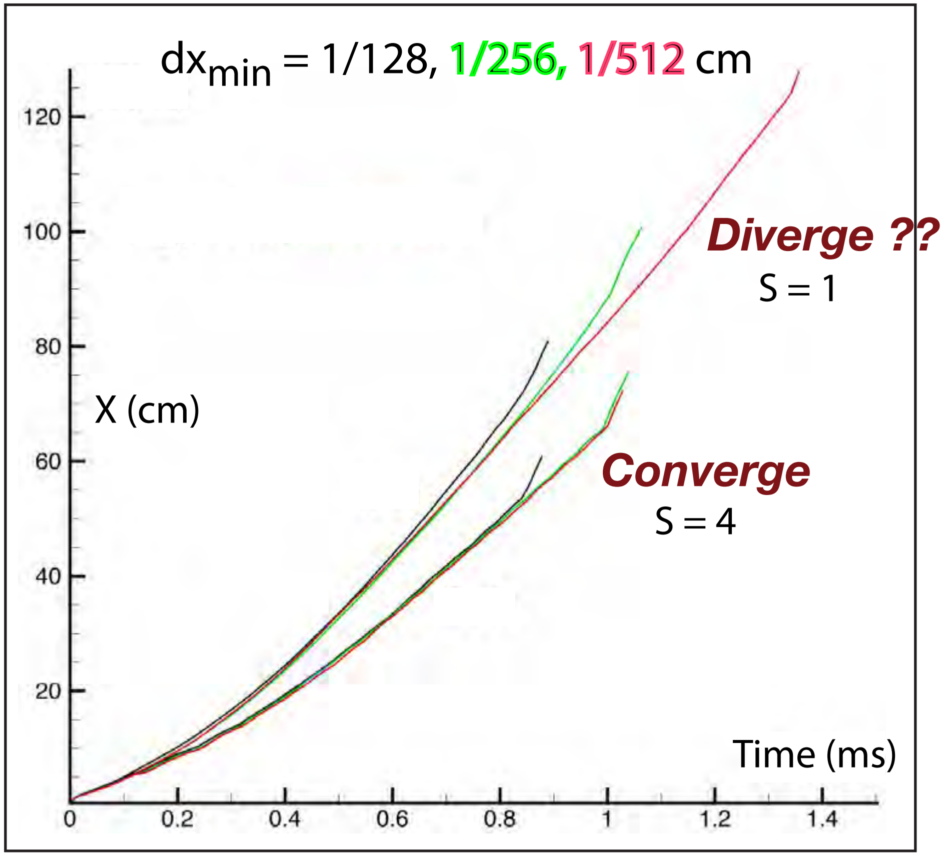
Shock-flame interactions are specific forms of the Richtmyer-Meshkov (RM) interaction -- the interaction of a shock and a contact surface.

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

If the fluctuations in the system are important, and the spectrum is dominated by RM, it could help explain the observations.

Resolution Tests ...





It appears as though S=4 case converges, but S=1 case cannot!

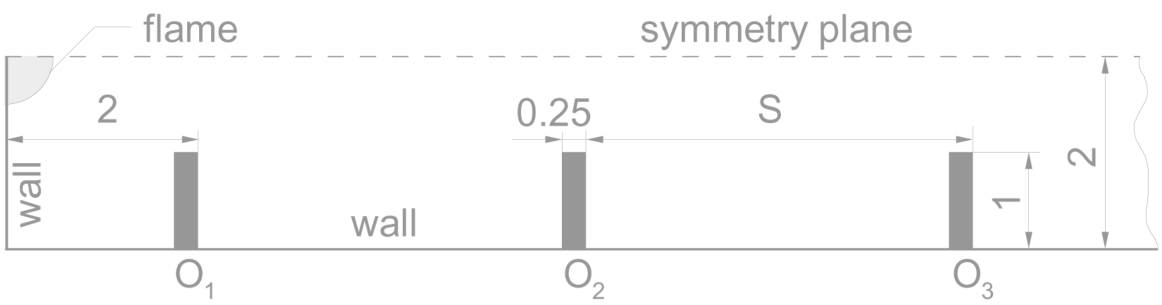
S -- space between obstacles

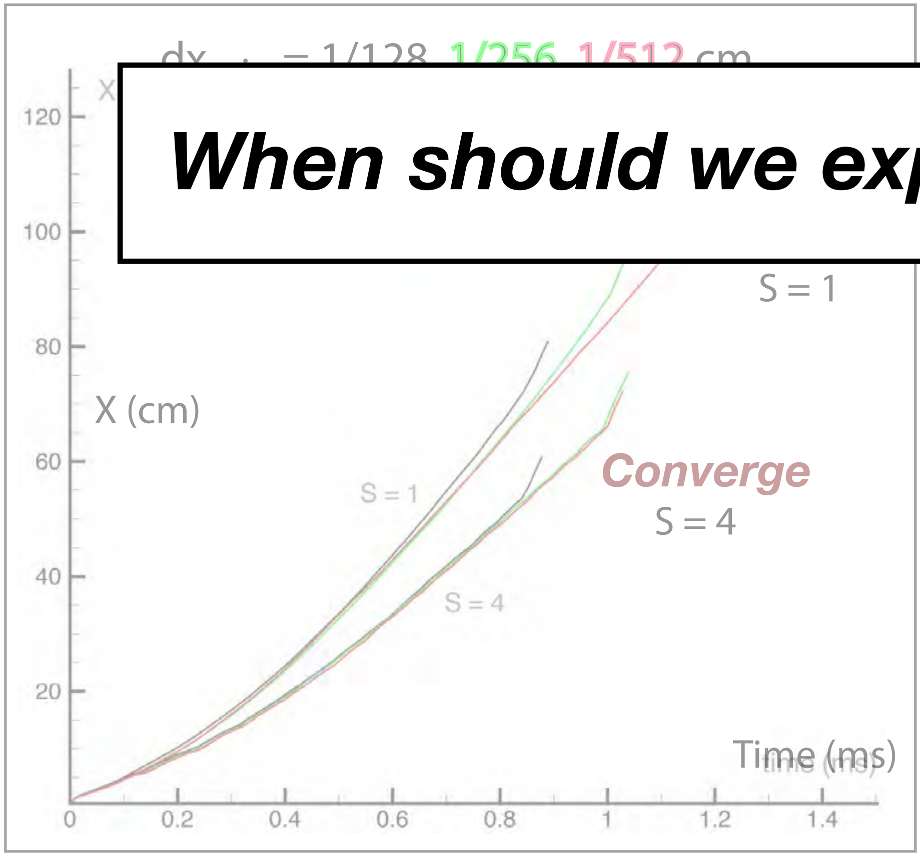
S = 1 -- DDT initiation by direct collision of incident shock and obstacle

S = 4 -- Mach stems important for DDT

Abilty to converge depends on the ignition mechanism ... ??

Resolution Tests ...





It appears as though S=4 case

!

When should we expect convergence??

S = 1 -- DDT initiation by direct collision of incident shock and obstacle

S = 4 -- Mach stems important for DDT

Abilty to converge depends on the ignition mechanism ... ??

Stochasticity

The ability of a process to deviate ramdomly from its path.

Turbulence is a stochastic process.

Experimentally, DDT occurs with some uncertainty in time and location. (Different physical regimes often have different levels of dispersion in the experimental result.)

This is the natural behavior of complex systems with multiple stochastic phenomena: turbulence and hot-spot formation

We can test this ....

Impose random perturbations in background initial conditions of $\Delta T = 0.01K$, look for dispersion in results.

Described by Gamezo et al. (CNF 2008; APS DFD 2009)

Stochasticity ...

A subject that needs
more work to translate into
meaningful physics and
guidelines for risk analysis ....

Where Do We Go from Here ... ??

Hot spots ... small, dynamic, control transition in the flow.

Turbulence ... how can the predictions be so good?

Stochasticity ... how can the predictions be so unreliable?

Thank you for your kind attention !