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AIRCRAFT TECHNOLOGY, CONVENTIONAL, STOL/VTOL

FLUID DYNAMICS

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A Special Issue to Celebrate Never-Published Papers

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COMPUTATIONAL FLUID DYNAMICS

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Complete Simulations in a Cord with Natural Flight: On the Wings of Angels

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Towards the Ultimate Conservative Scheme for Reconciling Mussel with Gherkin

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Approximate Indiscreet Solvers: The Importance of Being Upwind

Philip L. Roe
University of Michigan

AIAA Aerospace Sciences Meeting

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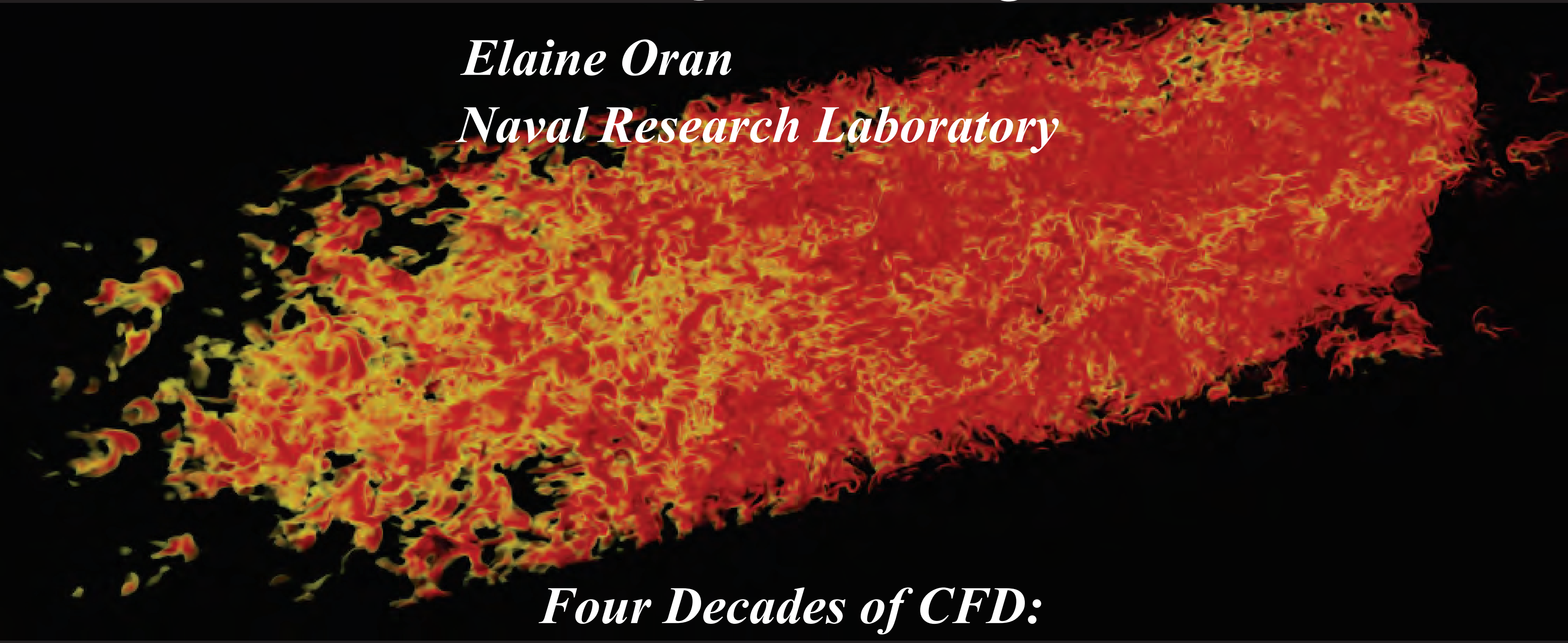
Concerns for Future Directions in Chemically Reacting Flows

Vadim

Looking Backward and Moving Forward
The JRV Symposium
San Diego, June 2013

Concerns for Future Directions in Chemically Reacting Flows



Elaine Oran
Naval Research Laboratory

Four Decades of CFD:
Looking Backward and Moving Forward
The JRV Symposium
San Diego, June 2013

To be able to use computers to learn about and -- with luck -- even predict the behavior of reacting flows, we need algorithms for:

Solving for the fluid dynamics -- CFD,

and ways to represent

Chemical transformations -- ODEs ?, other?

and the technology to combine these.

Antony, Bram, and Phil are among those who have have provided some of the basic underpinnings of modern CFD.

Reactive Flows

Flows with localized reactions and energy release

"... encompass a very broad range of phenomena, including flames, detonations, chemical lasers, the earth's atmosphere, the Sun, stars, supernovae,...

Despite the obvious physical differences among these flows, there is a striking similarity in the forms of the descriptive equations. Thus the considerations and procedures for constructing numerical models of these systems are also similar."

***Now consider some reactive flows
at very different scales ....***

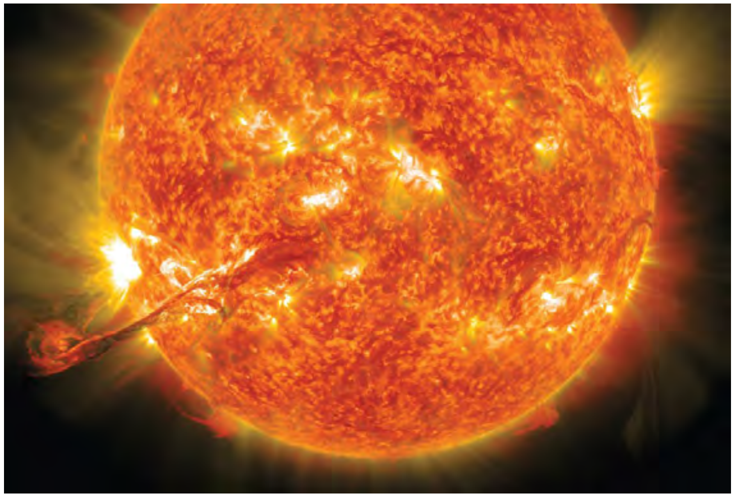
Galaxy NGC4536

Type Ia Supernova, ... 1981B

Released ~ 10^{51} ergs in 2s

Some Reactive Flows of Current Interest

Coronal Magnetic Eruption 2012



Wildfires ... Colorado 2012

Aircraft explosion 2008

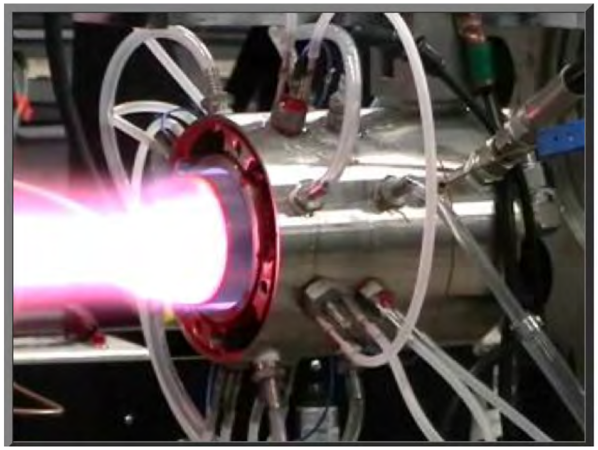
Mine Explosion Greymouth, 2010

Flows are energetic, unsteady, high-speed, turbulent.

Buncefield, UK
5 December
2005

Why was there such extensive damage?

Rotating Detonation Wave Engine



Annulus perpendicular to an inlet and nozzle system. Incoming propellents are continuously ignited, and detonate, producing thrust. (Courtesy UT Arlington)

Scramjet Engine

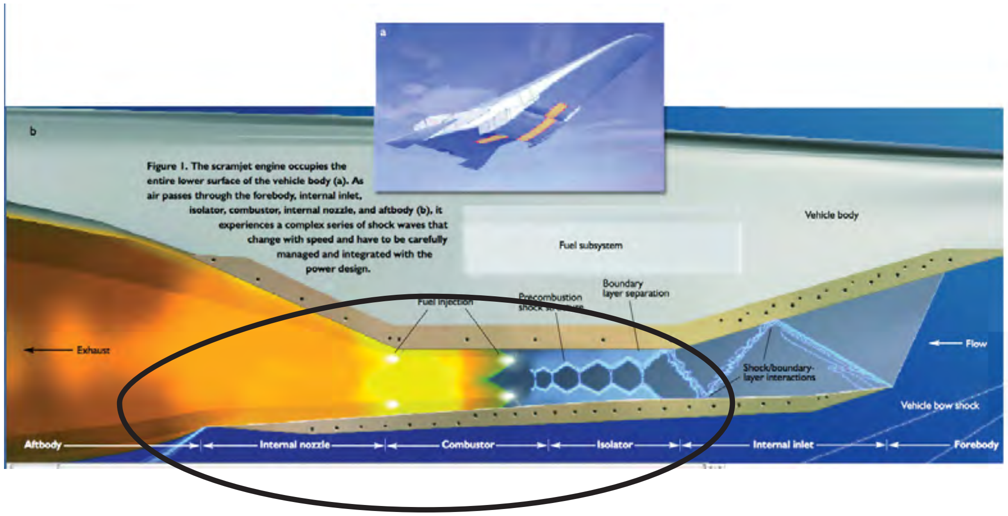
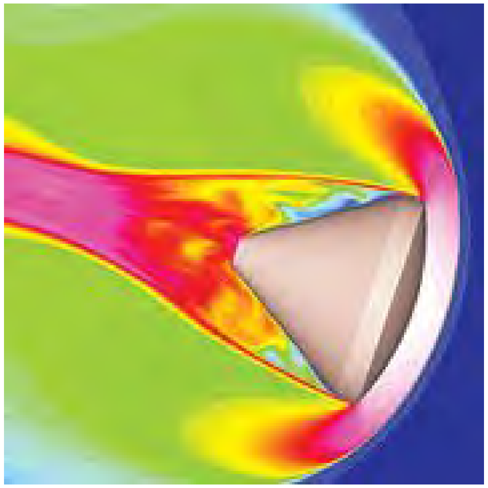


Figure 1. The scramjet engine occupies the entire lower surface of the vehicle body (a). As air passes through the forebody, internal inlet, isolator, combustor, internal nozzle, and aftbody (b), it experiences a complex series of shock waves that change with speed and have to be carefully managed and integrated with the power design.

Atmospheric Reentry Flow



Summary of Concerns

For fast and variable flow with intense energy release ...

We don’t know if the fluid equations hold.
We know the chemical mechanisms are wrong.
(And this says nothing about the other terms.)

Lament:

“So it seems to me that the underpinnings are … weak, weakening? I had thought that reacting flows were on fairly solid ground. There are some rumbles now, which could turn into earthquakes.”

Reply:

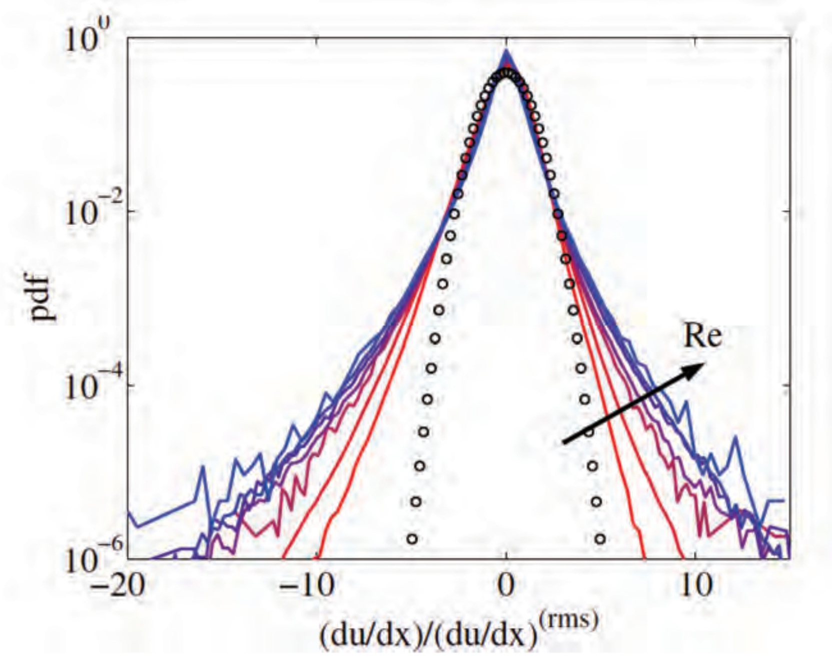
“I don't think they are weakening, I think they were never strong. It may be that some people are realizing for the first time how weak the underpinnings are. I hope this does not lead people to jump in off the deep end. ‘Petit a petit l'oiseau fait son nid.’ Slow and steady is what we want.”

Intermittency

"Occurring at irregular intervals; not continuous or steady"

There are several meanings of "intermittency" in turbulence.

First, consider one of them, "the tendency of the probability distributions of some quantities in 3D turbulence (i.e., gradients or velocity differences) to develop extreme tails at the wings."



Pdfs of longitudinal velocity gradient for several values of *Re*, ***increasing in direction of the arrow. Normalized by the standard deviation. Symbols are Gaussian.***

(Jimenez et al., 1993; Belin et al., 1997; Antonia and Pearson, 1999)
(Re in range 260 - 3.5x10^6)

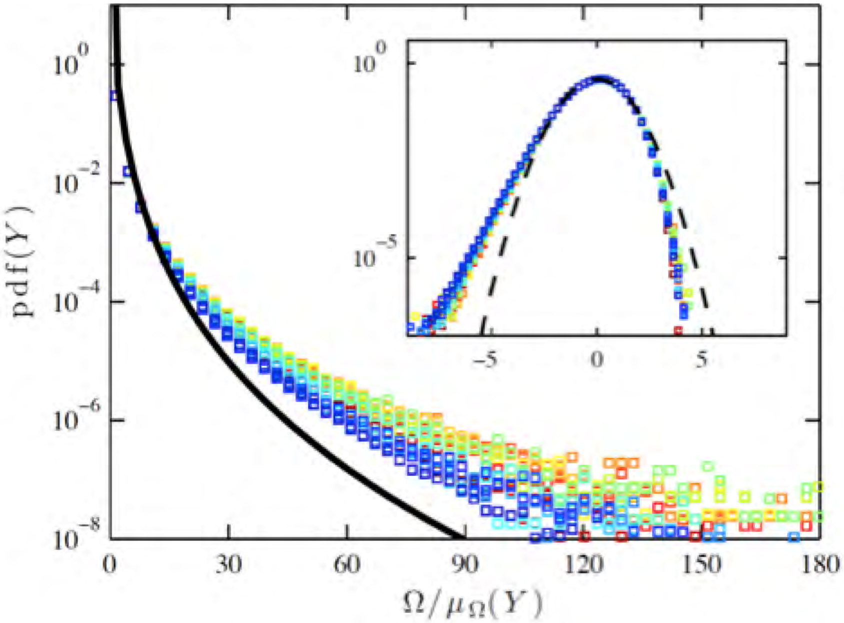
* ***These tails become stronger as the*** *Re* ***increases. (This means that fluctuation level increases.) The effect does not show any sign of stopping at the highest*** *Re's* **.**

Intermittency in Turbulent Reacting Flows

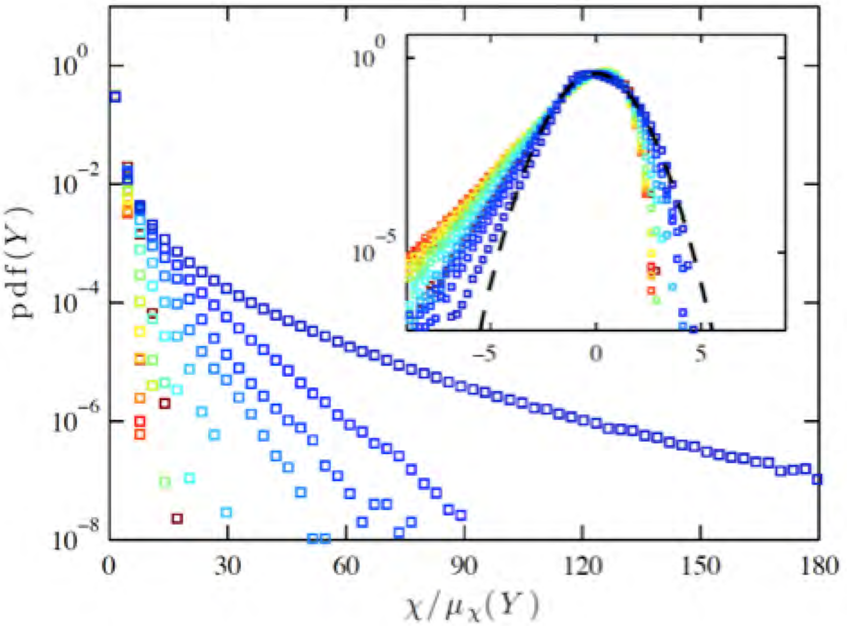
How do variations in turblent intensity (I_T) affect fluctuations of flow variables?

Turbulent flows and flow variables show intermittency, here quantified (by pdfs) as deviations from Gaussianity.

Enstrophy (vorticity Ω)



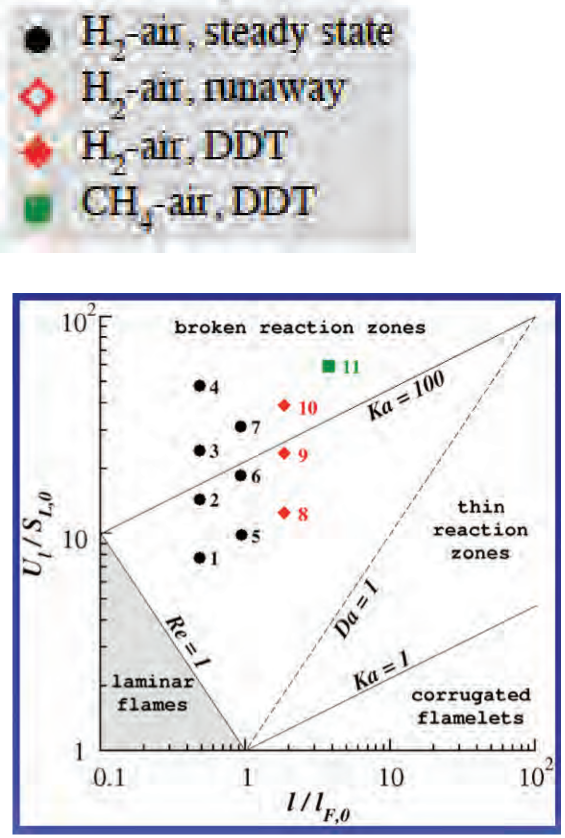
Scalar Dissipation (χ, i.e., grad Y)



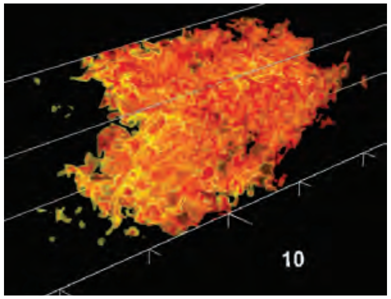
(Key: Y = 1, blue, unreacted   Y = 0, red, reacted
Log-normal modelis in the inset.)

What does intermittency mean for us practically?

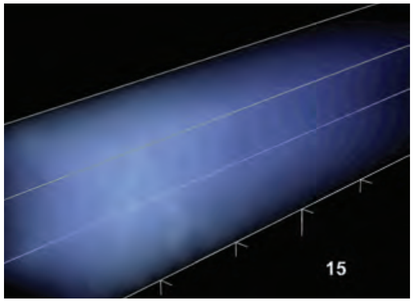
Fluctuatons in physical variables (P, T, v, ...) can have dramatic effects in an exothermic material.

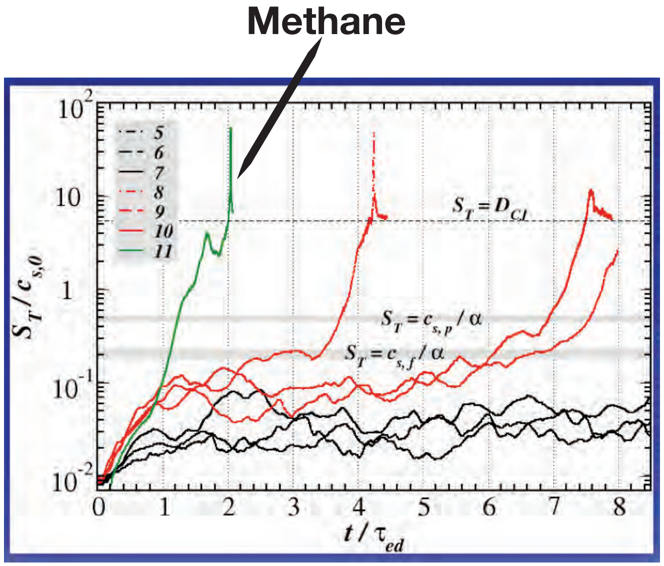


Fuel Mass Fraction



Pressure





One thing we know: there is more chance of an extreme event, a large and strong effect in the flow, to occur as Re increases.

Reasons for Worrying about Intermittency

Intermittency can affect the likelihood of
extinction, re- and auto-ignition, DDT,
instantaneously broaden or thin flames, and
produce other extreme configurations

Intermittency strongly varies both with turbulent intensity and fuel mass fraction (position in the flame)

Turbulence (enstrophy, energy dissipation) is more intermittent for small intensities, particularly near products

Scalar dissipation is more intermittent for high intensities, especially near reactants

Intermittency increases with Re, T, ...

Issues with Standard Chemical Reaction Mechanisms

- **Complex hydrocarbons (e.g., biofuels, JP's, gasoline, ...):**
  Chemical reaction mechanisms with ~10^4 chemical reactions are common. Mechanisms with ~10^5 and even more reactions now proposed.
  - ***Assumptions:***
    - **Equilibrium kinetics mechanisms.**
    - **Specific reactions intermediates.**
    - **Sequential steps represented by Arrhenius rates.**
    - **Rates and other input are guesses, extrapolations, fits.**
    - **Many unknown parameters.**

- **None of the proposed mechanisms (even hydrogen alone) consider high-T,P conditions, or the presence of shocks.**
  Shocks put molecules into nonequilibrium excited states, and these can be the states undergoing reactions.

- **Civil Asides: (1) At any location in space and time, very few of these Arrhenius reactions and species are important.**
  (2) In the course of the reaction, excited states of short-lived intermediates (known and unknown) can be critical.

Test of a Chemical Reaction Mechanism

When combined with a fluid model, does it reproduce the “cleanest” measurements we can make?

- ***Laminar flame speeds***
- ***Flame instabilities***
  (e.g., multidimensional cellular structure)
- ***Detonation velocities (and variation on mean)***

- ***Multidimensional detonation structure (structure & size)***

This is where the algorithms that Jay, Bram, Phil and Antony have allowed us to compute accurately enough to be quantitative.

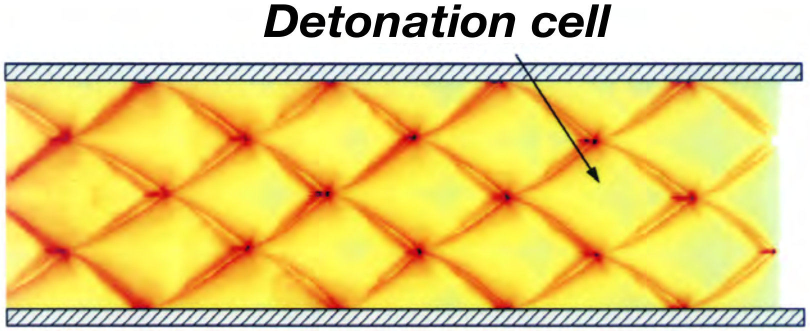
This is where the chemical models fail badly, both qualitatively and quantitatively.

Detonation Cells as a Test of Chemical Kinetics for High-Temperatures, High-Pressures

Early computations of cellular detonation structure using detailed chemical reaction models: e.g.,

Oran, Weber, et al. ~1998: 2D simulations of structure of detonation cells for low-pressure H_2-O_2, with Ar (~70%).

Computed and measured cell sizes were similar (within factor of 2).



Repeated more recently by *Eckett (2001)*, *Hu et al. (2004)*, and *Dieterding (2011)*, with more resolution, updated chemical models, etc. *Computed and measured cell sizes still similar.*

Conclusion: For low-pressure, strong dilution (Ar, N_2) , computed cell sizes are generally within a factor of 2 of measured cell size. Structure looks OK.

Most Recent Detonation Cell Computations:

H_2-air, 1 atm, 298K (*Taylor et al., 2011-12)*

**1-step, 12-step, 24-step, GRI-Mech, UCSD, ...
models, all fairly "standard" chemical models.**

4 different high-resolution numerial fluid dynamics methods.

***Result:* All mehanisms, with any numerical method, give computed cell sizes ~0.01 m, i.e., ~5-10 too small.**

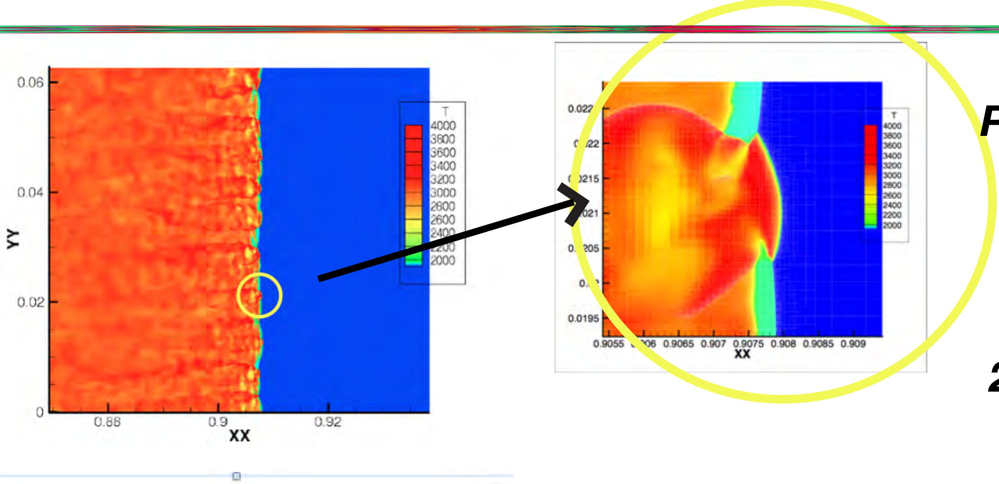
(*Burke et al.* high-pressure chemical model gives cell sizes ~4-5 times too small.)

Computed cell structure (i.e., regularity, shape) is also wrong!

Why???

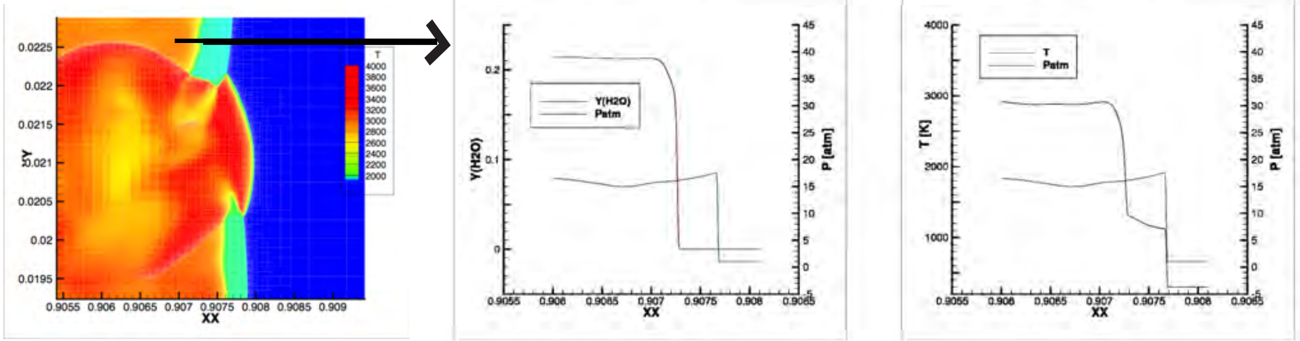
This same trend for computed cell sizes is echoed in measurements and simulations of detonation cells for CH_4-air, 1 atm, 298 K (Kessler et al.).

Reactive Flows under Extreme Conditions

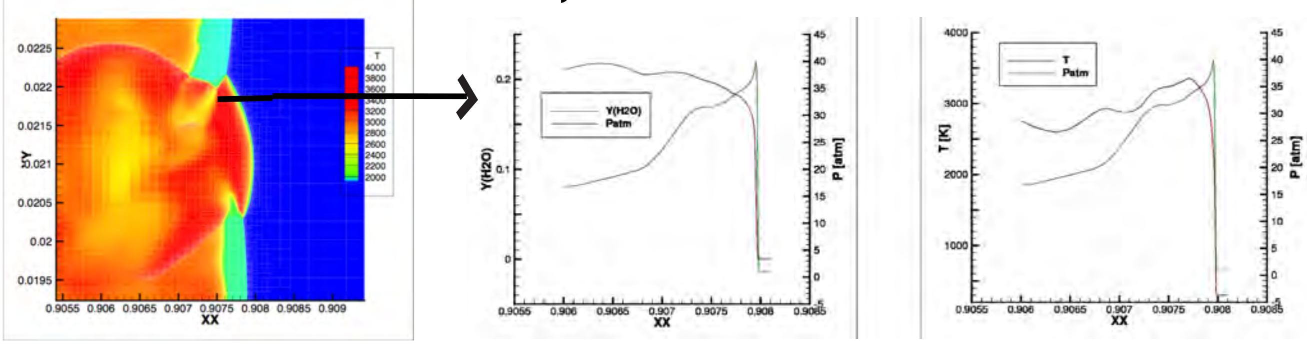


Propagating detonation in H_2-Air, 1 atm, 298K. Burke et al. chemistry. Computations by Taylor, Kessler et al., 2011-12 (Proc.Comb.Inst).

Post-Shock State: 18 atm, 1100 K



Post-Shock State: 40 atm, 2200 K



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Thank you for your kind attention !