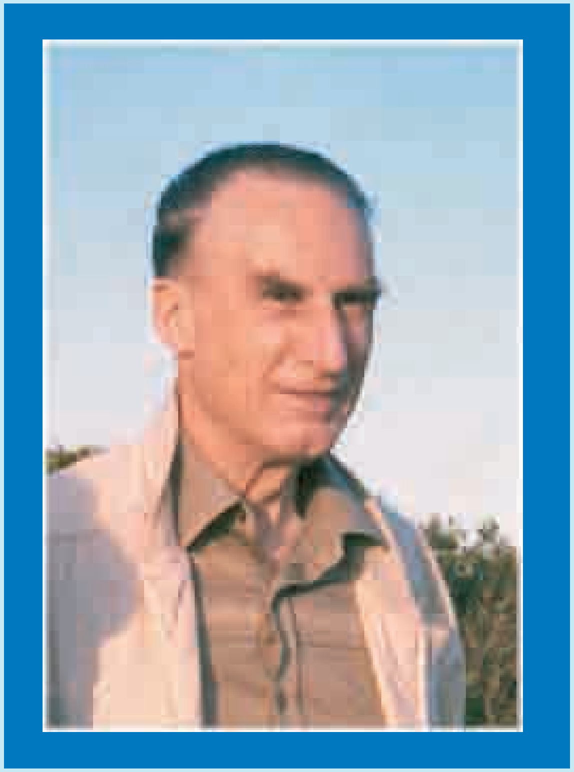
Tales of Detonation
Initiation, Propagation, and Quenching

A Tribute to Huw Edwards

Elaine S. Oran
Naval Research Laboratory
Washington, DC

50th UKLEG Anniversary Meeting
Explosion Safety - Assessment and Challenges
Cardiff, July 2013

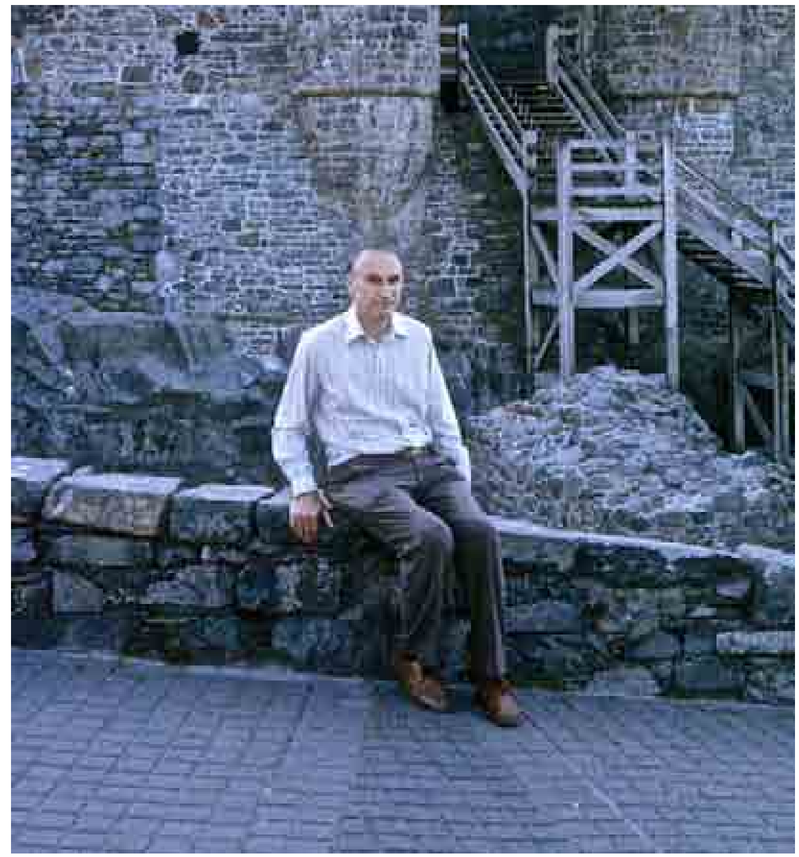
D. Huw Edwards
University of Wales Aberystwyth



(1925 ?? - 2003)

"... among the giants of gasdynamics worldwide..."

"... an innovative experimentalist with a deep understanding of theory..."



(1985)

Memories of the Past
Comments on the Present
Thoughts for the Future

Vadim

Memories of the Past

Vadim

Detonation Structure and Dynamics

18th International Combustion Symposium
University of Waterloo, Canada, 1980

"Numerical Simulations of Detonations in Hydrogen-Air and Methane-Air Mixtures"

We showed this picture, but it had not appeared in the accepted paper.

Was it a "real phenomenon" or a numerical artifact ???

It was the only topic of the discussion!

578 DETO

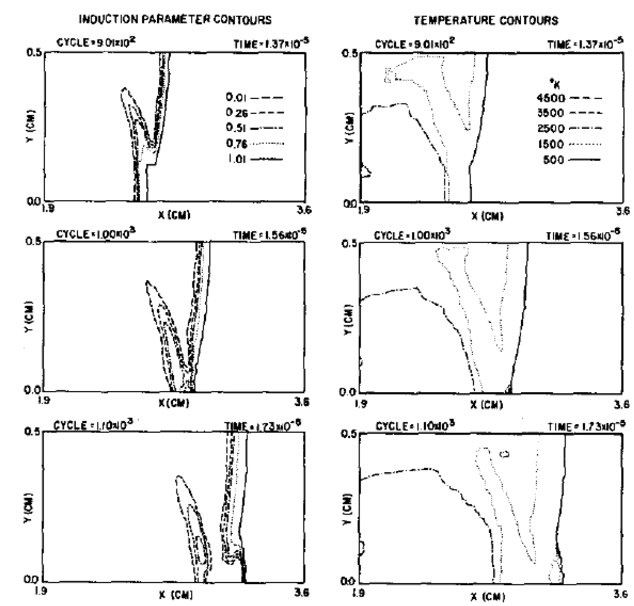


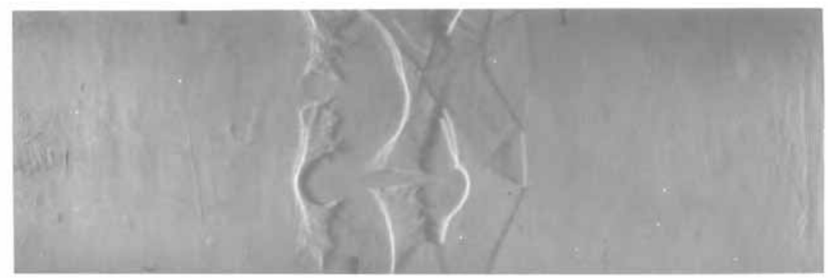
FIG. 6. Temperature and induction parameter contours from a calculation for the same mixture as in Figs. 3, 4, and 5 except in a tube 0.5 cm high.

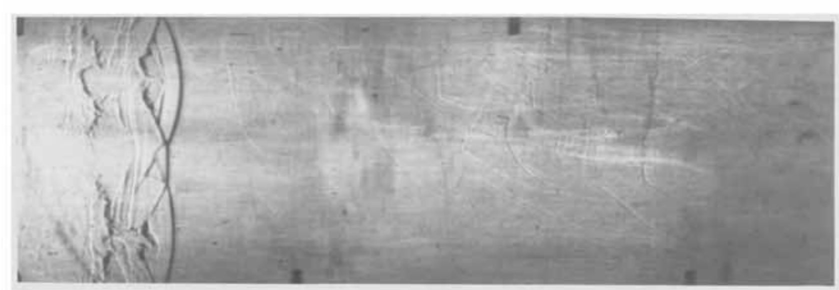
Detonation Structure and Dynamics

"I saw something like that in marginal detonations and so did the Russians in Siberia, but we swept it under the rug."

"Here are some that I found for you ... "

Provided by Huw ...
Produced in early '70's





Detonation Structure and Dynamics

V.A. Subbotin, 1975

"Two Kinds of Transverse Wave Structures in Multifront Detonation"

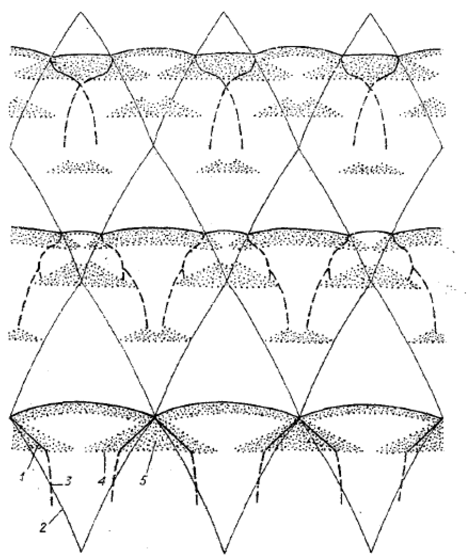


Fig. 3. Idealized diagram of the process of detonation propagation with transverse waves without a reaction. 1) Shocks in the unburned gas; 2) trajectories of triple-point motion; 3) compression waves in the burning gas; 4) combustion fronts; 5) unburned gas.

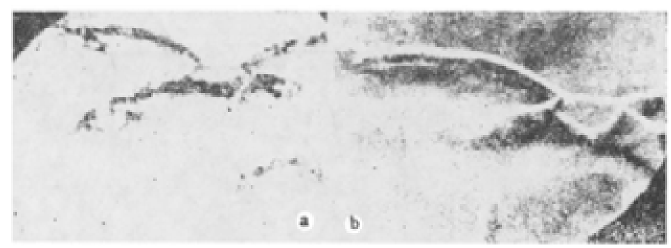
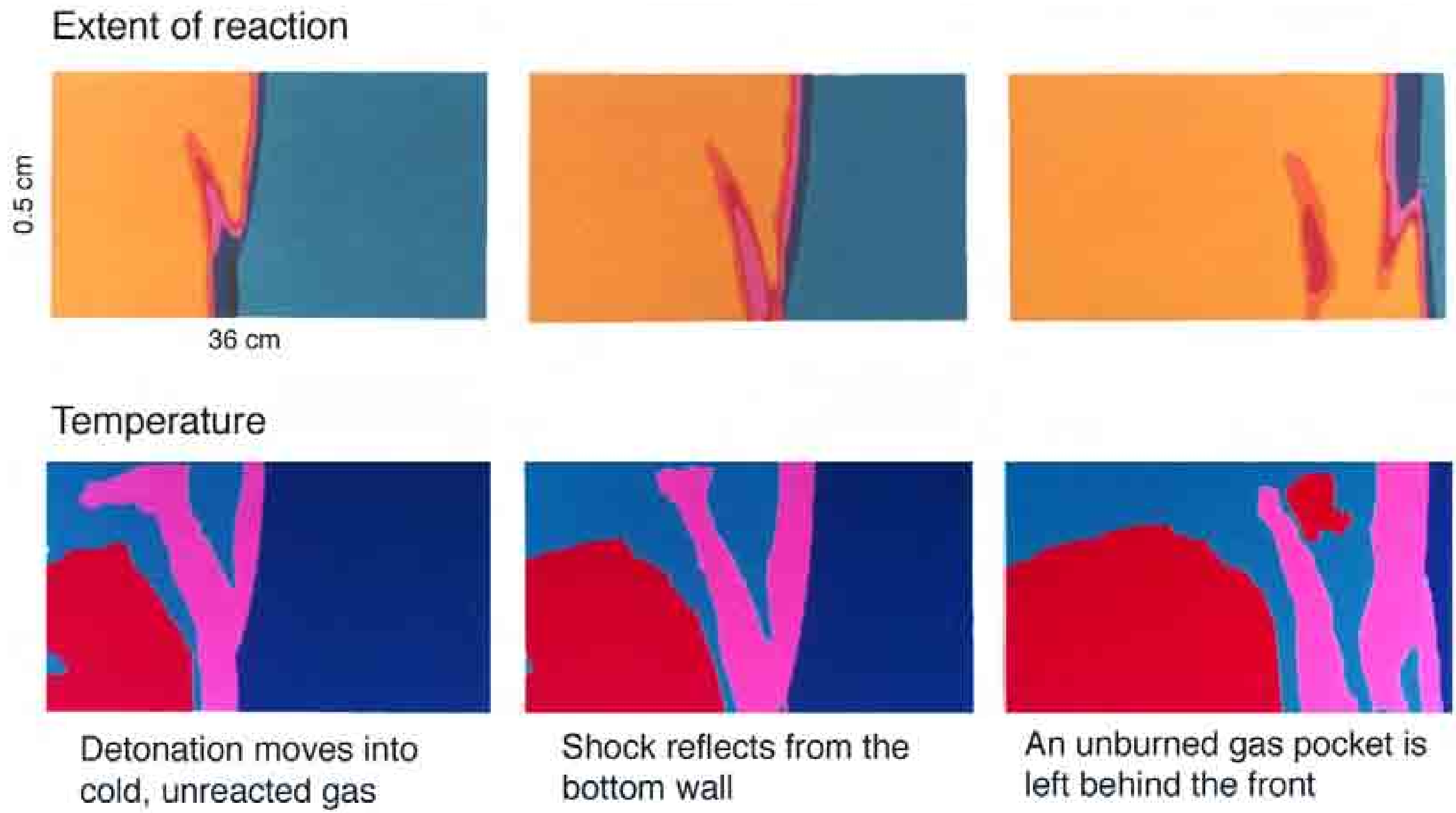


Fig. 4. Waves of type II in a mixture of $CH_4 + 2O_2 + 6\%$ air, $p_0 = 80$ mm Hg (a) and waves without reaction in a $2H_2 + O_2$ mixture (wave of type I on the right and of type II on the left, $p_0 = 70$ mm Hg) (b).

And here they were again, ... in 1975

Detonation Structure and Dynamics

19th International Combustion Symposium
Haifa, Israel,1982

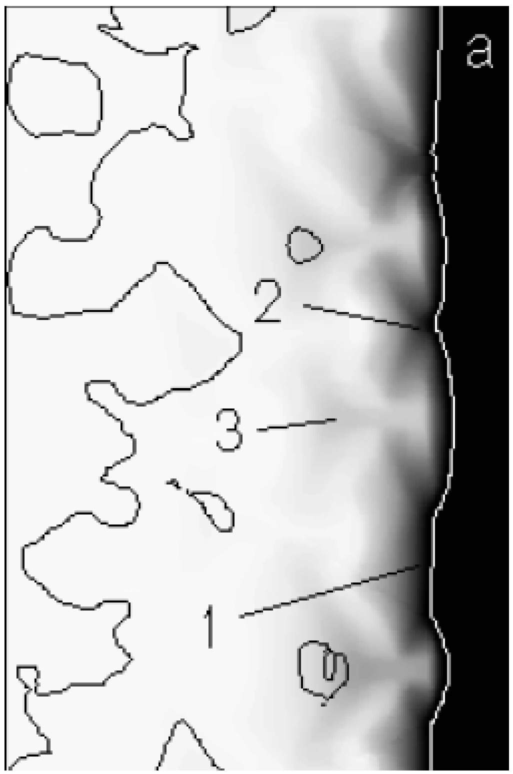


"A Study of Detonation Structure: The Formation of Unreacted Gas Pockets" - Discussions as possible mechanisms of detonation ignition, reignition, propagation, extinction ... Figure appeared in Scientific American.

"Keystone" Features

Computation

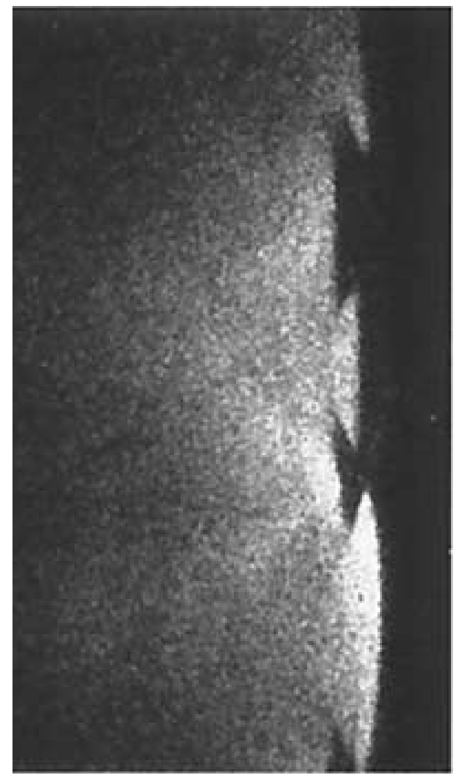
low E_a/RT_s



V.N. Gamezo, D.Desbordes, E.S.Oran 1999

Experiment

H_2/O_2 + 85% Ar

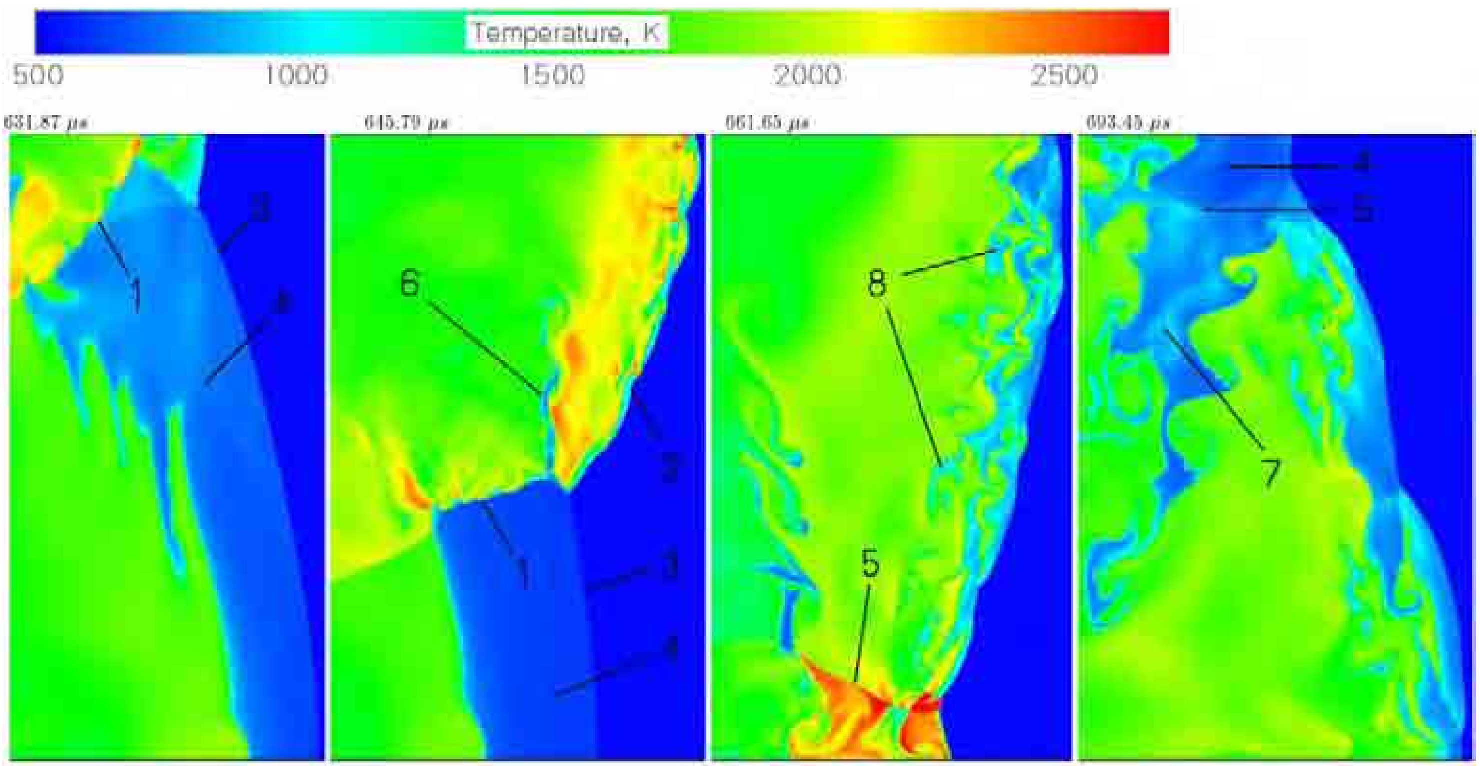


F. Pintgen, C.A. Eckett, J .M. Austin, J.E. Shepherd 2003

Detonation Structure and Dynamics

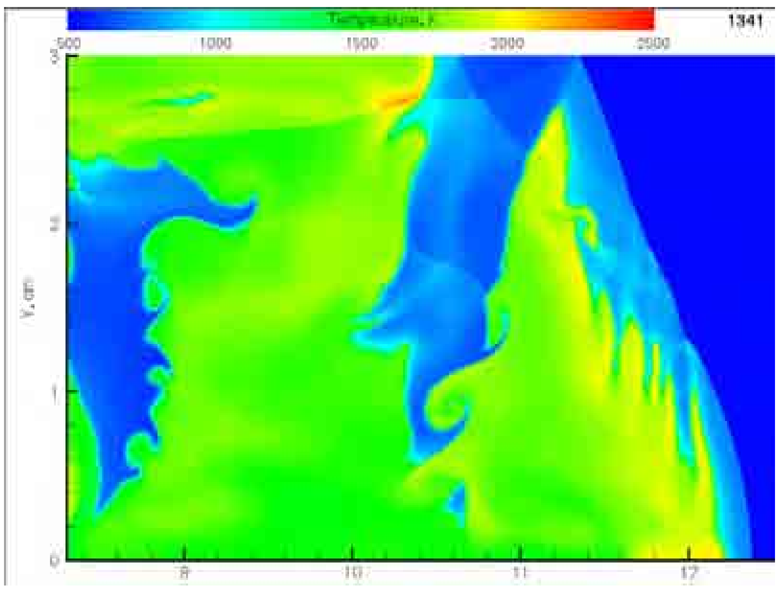
28th International Combustion Symposium
Edinburgh, Scotland, 2000

“Fine Cell Structure Produced by Marginal Detonations”
(Gamezo et al.)

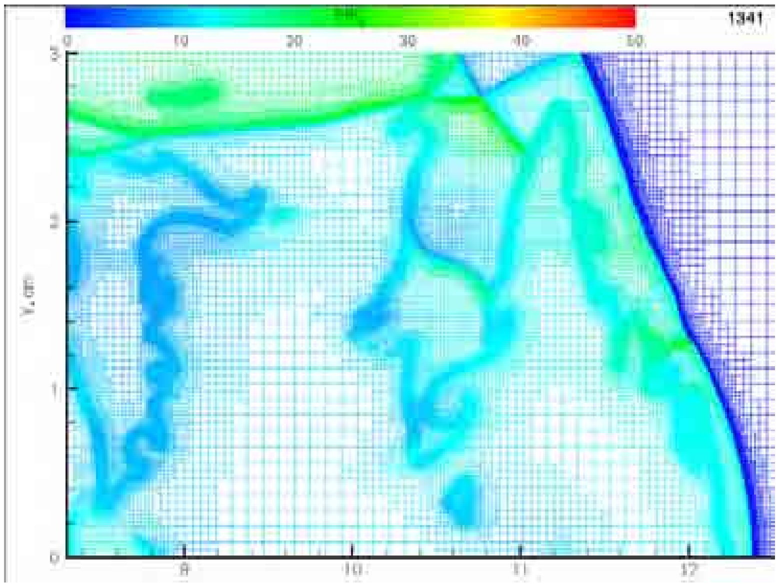


1 - Transverse detonation
2 - Strong part of the leading shock (overdriven detonation)
3 - Weak part of the leading shock (inert)
4 - Induction zone
5 - Transverse shock
6 - Unreacted tail
7 - Primary unreacted pocket
8 - Secondary unreacted pockets

Temperature

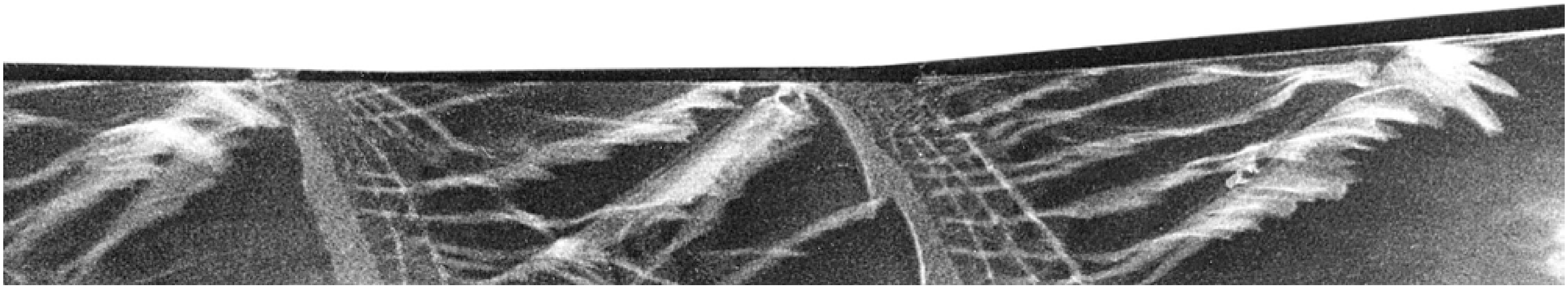


Pressure and Grid

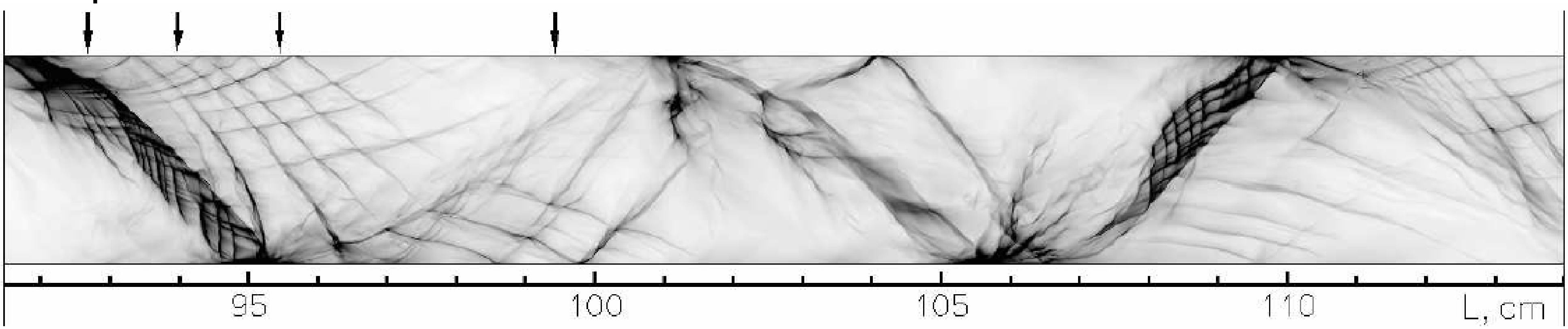


Fine Cellular Structures

Open-shutter photograph by A. A. Vasil’ev



Computed smoke-foil



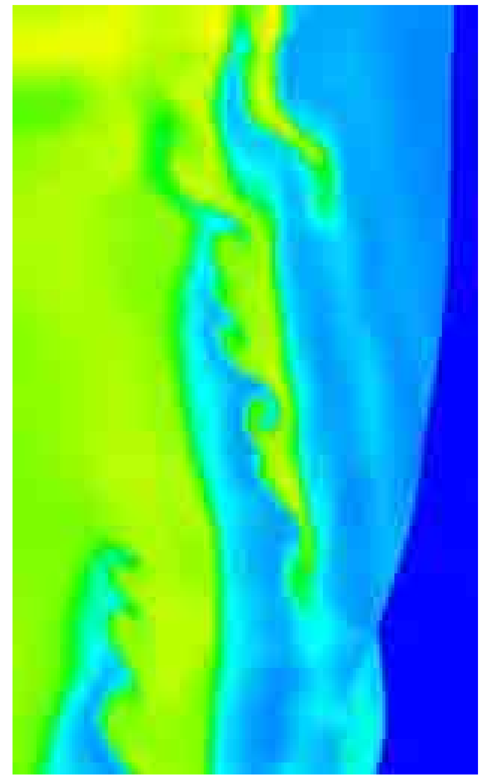
Marginal detonation in $C_2H_2 + 2.5O_2$ in flat channel

Kelvin-Helmholtz Instability

Experiment

F. Pintgen, J .M. Austin,
J.E. Shepherd 2003

Computation



V.N. Gamezo, A.A.Vasiliev,
A.M.Khokhlov, E.S.Oran 2000

Features of Pockets -- what we learned

Natural part of detonation cells. Become larger as approach limits.

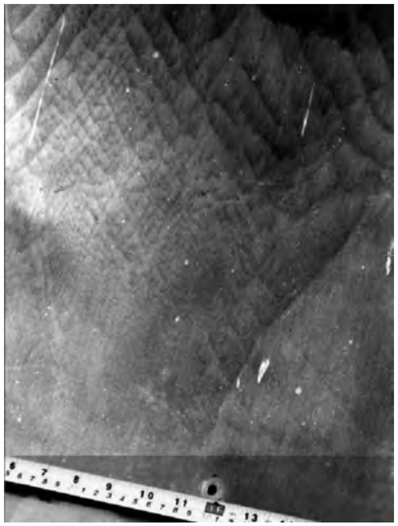
Could lead to detonation extinction.

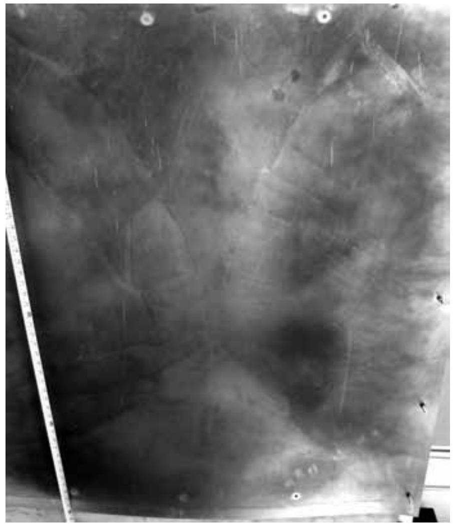
Most obvious when there are large reaction zones behind the detonation front. Result as shocks interacts with reaction zones.

When pockets are very large (as approach limits, spinning detonation), secondary detonations can propagate in large reaction zones. These a can be very powerful.

Detonation Structure and Dynamics

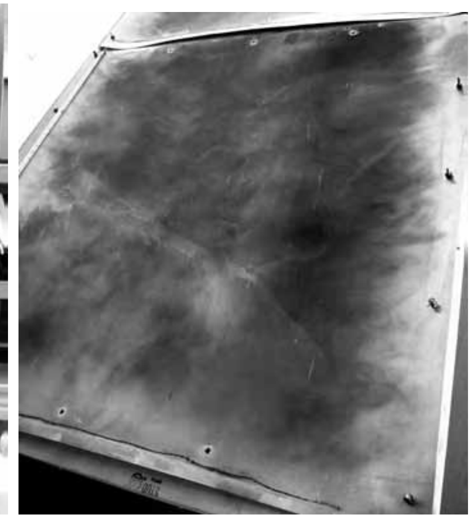
Secondary Detonation Cells





6.2% CH_4   *5.5% CH_4*

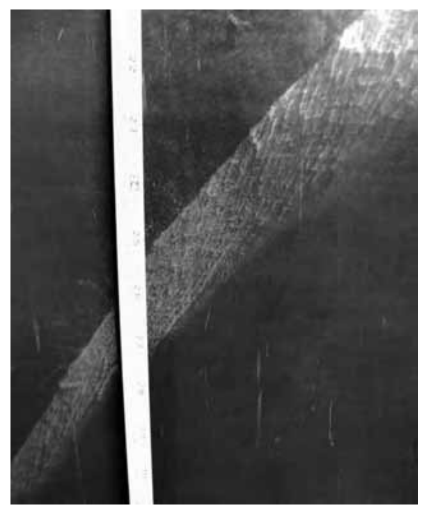
Traces of Spin Detonation



5.3% CH_4   *15.5% CH_4*

Fine Detonation Cells inside Spin Traces

Lake Lynn, GETF ~ 2008



20 cm

14 cm

Comments on the Present

Vadim

Comments on the present ...

Our ability to compute realistic-looking scenarios describing combustion and explosion events has progressed enormously since we first started using computers to do this.

This results from the confluence of investments in large, multi-processor high-speed computers, lots of computer memory, new algorithms, and from the developing recognition of the importance of being able to compute, with some confidence, the properties of highly complex, nonlinear systems.

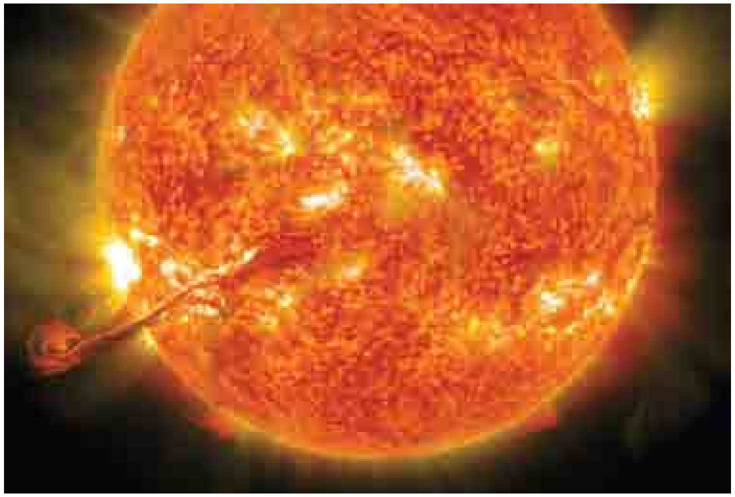
So that we can compute and maybe even predict DDT. Sometimes, the answers might even look correct.

More often, we can use the computations to understand trends and physical mechanisms.

For example, ...

Some Reactive Flows of Current Interest

Coronal Magnetic Eruption 2012



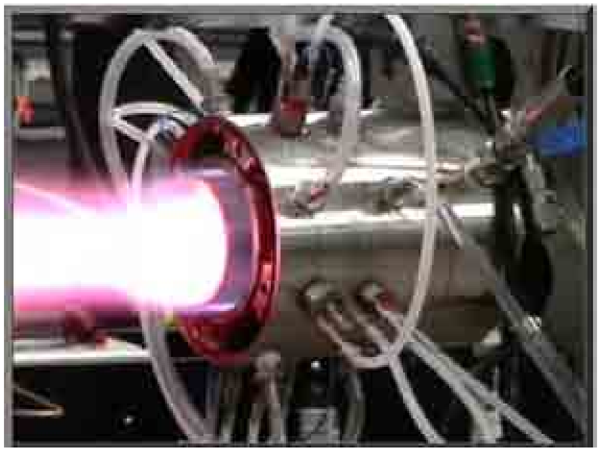
Wildfires ... Colorado 2012

Aircraft explosion 2008

Mine Explosion Greymouth, 2010

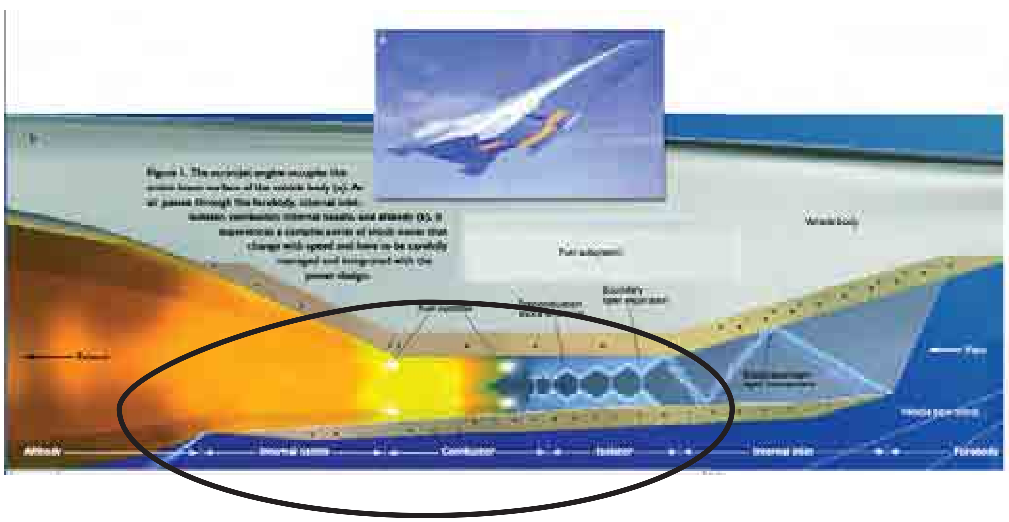
Flows are energetic, unsteady, high-speed, turbulent.

Rotating Detonation Wave Engine

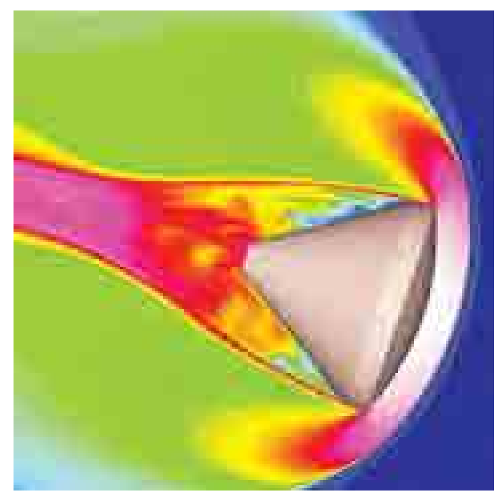


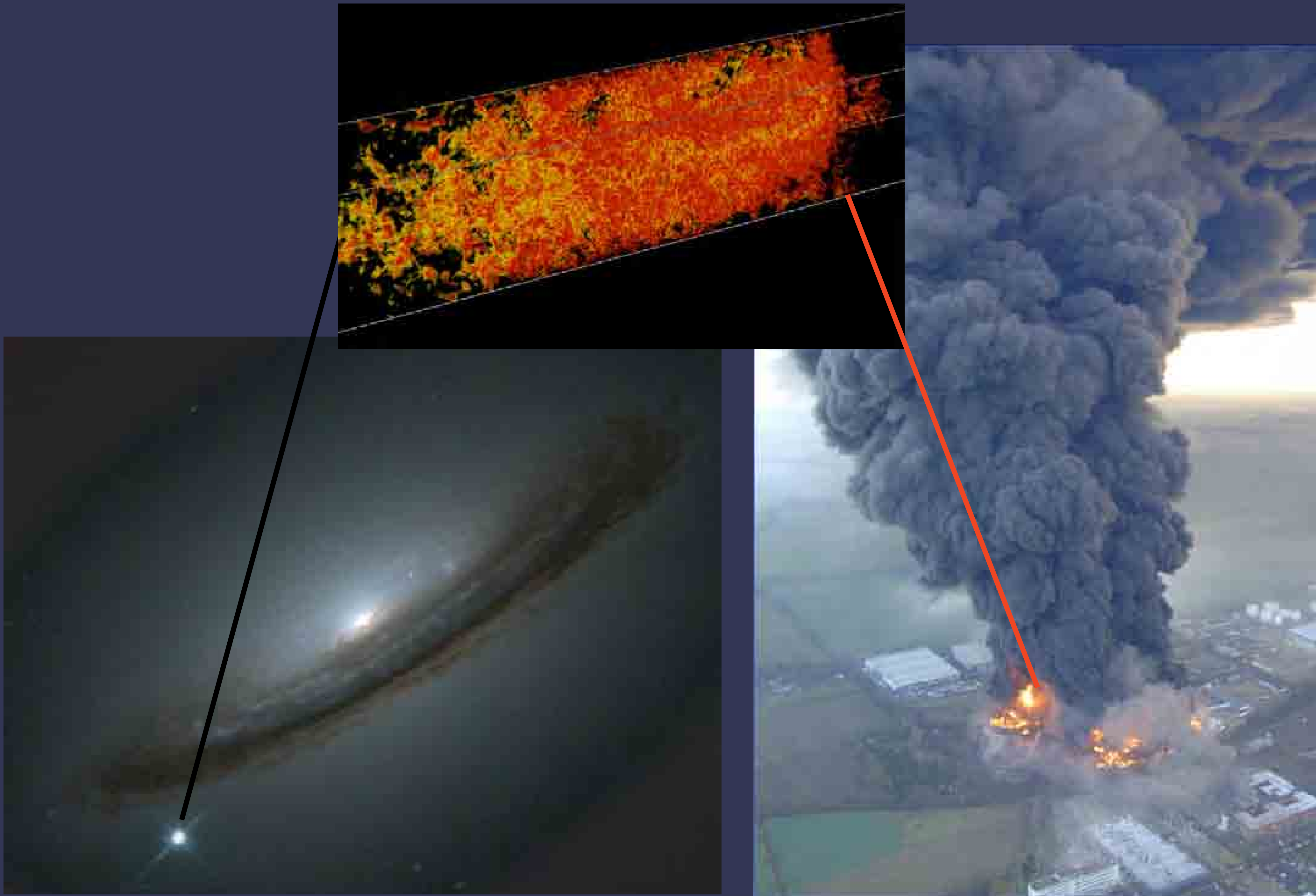
Annulus perpendicular to an inlet and nozzle system. Incoming propellents are continuously ignited, and detonate, producing thrust. (Courtesy UT Arlington)

Scramjet Engine



Atmospheric Reentry Flow





Thoughts for the Future

Vadim

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 physical processes.)

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:

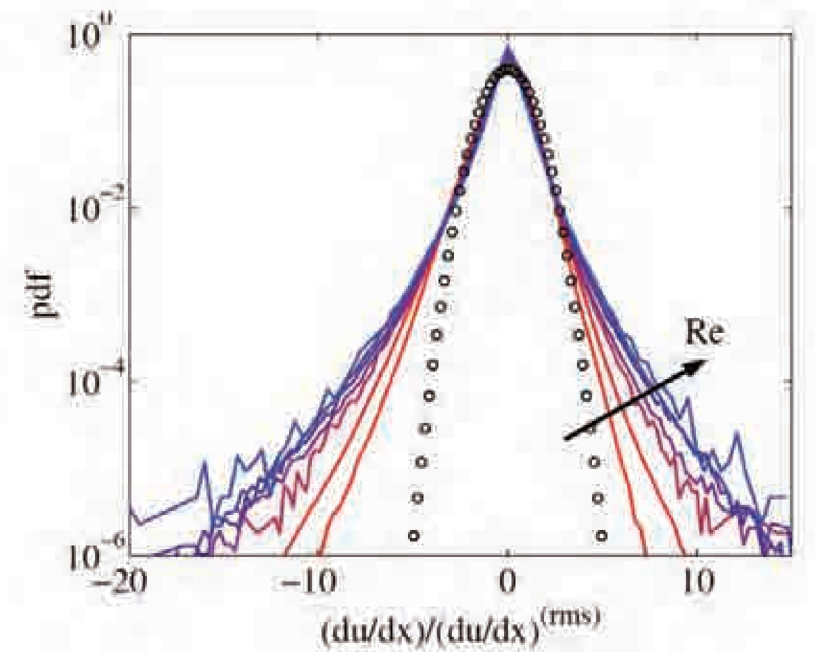
"I don't think they are weakening, I think they were never strong. It may be that some people are realizing for the first time how weak the underpinnings are. I hope this does not lead people to jump in off the deep end. 'Petit a petit l'oiseau fait son nid.' Slow and steady is what we want."

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* ***.***

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

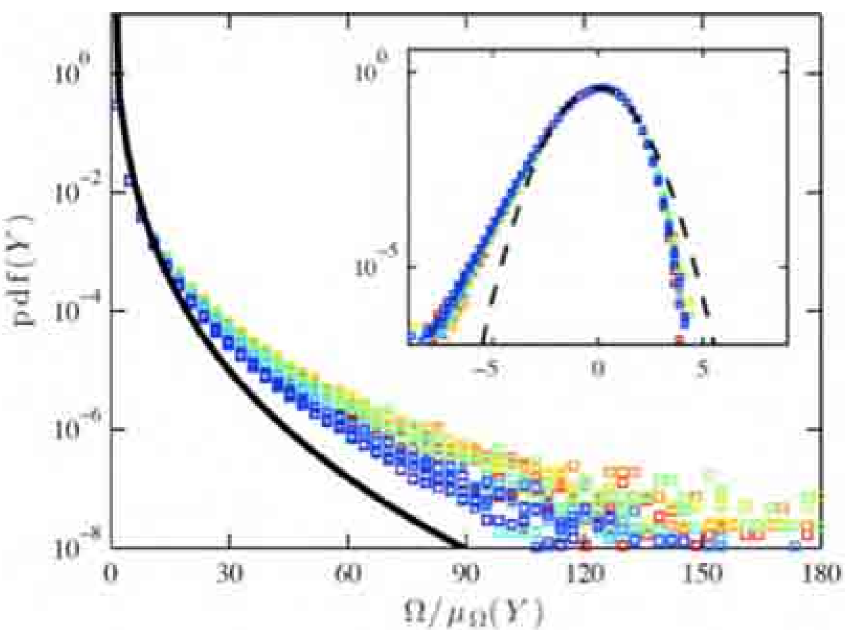
Intermittency increases with Re, T, ...

Intermittency in Turbulent Reacting Flows

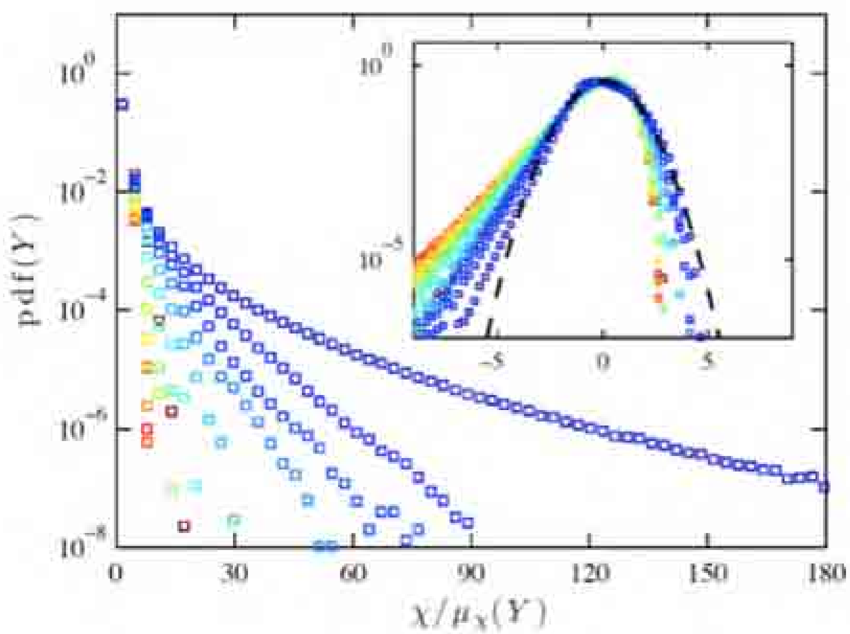
How do variations in turblent intensity (I_T) affect fluctuations of flow variables?

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

Enstrophy (vorticity Ω)



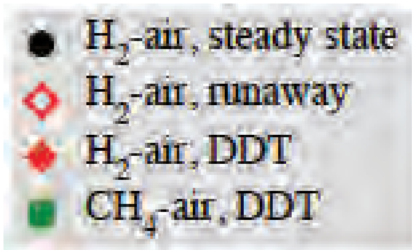
Scalar Dissipation (χ, i.e., grad Y)

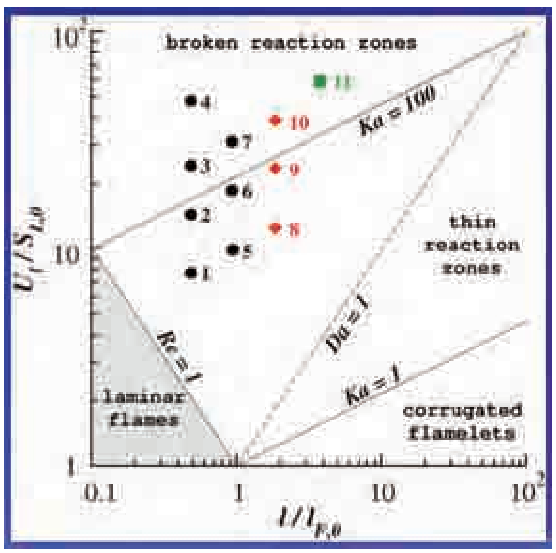


(Key: Y = 1, blue, unreacted   Y = 0, red, reacted
Log-normal modelis in the inset.)

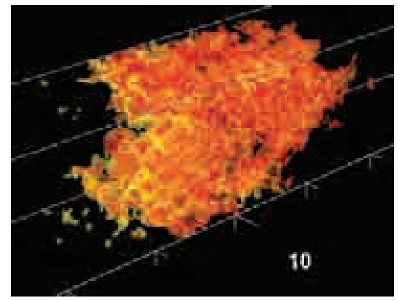
What does intermittency mean for us practically?

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

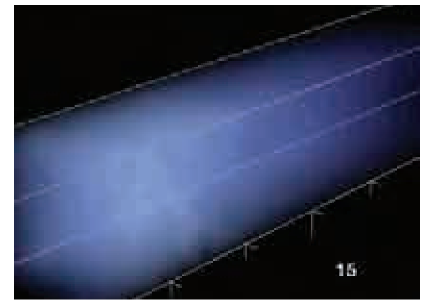




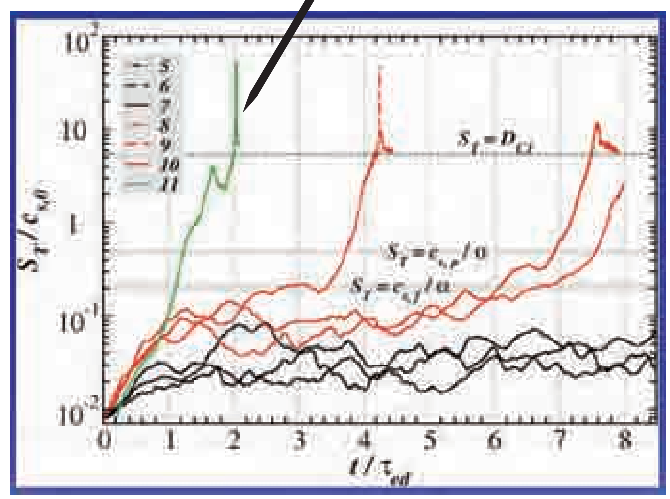
Fuel Mass Fraction



Pressure



Methane

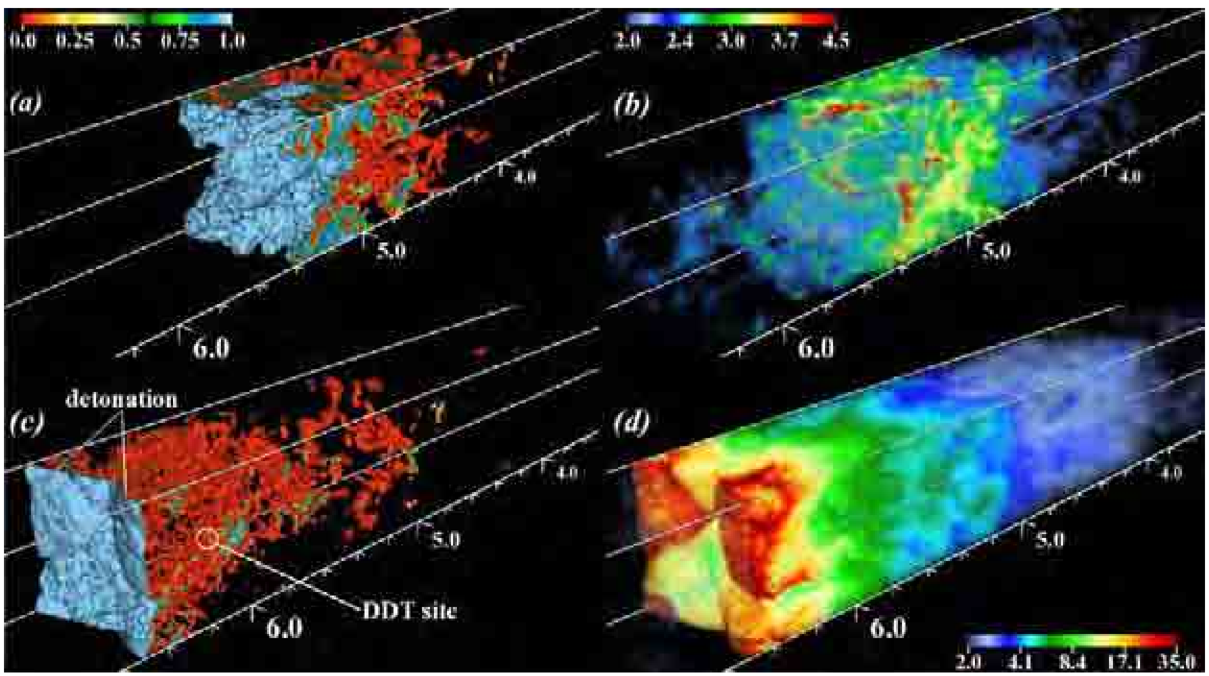


One thing we know: there is more chance of an extreme event, a large and strong effect in the flow, to occur as Re increases.

DDT Can Occur "Spontaneously"

For higher-intensity turbulent-flame interactions, detonations can arise "spontaneously."

A detailed analysis of one H_2-flame simulation showed that the transition was preceded by a large increase in the flame-brush pressure, resulting from intense turbulent-flame interactions. At that point, the entire flame brush accelerated to the CJ flame speed, shocks began to form locally inside the flame brush, and a DDT occurred inside the flame flame brush.



$$S_T = \frac{c_s}{(\rho_f/\rho_p)}$$

$$= S_{CJ}$$

(Poludnenko, Gardiner, Oran, PRL, 2011, Science (Editor's Choice))

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)

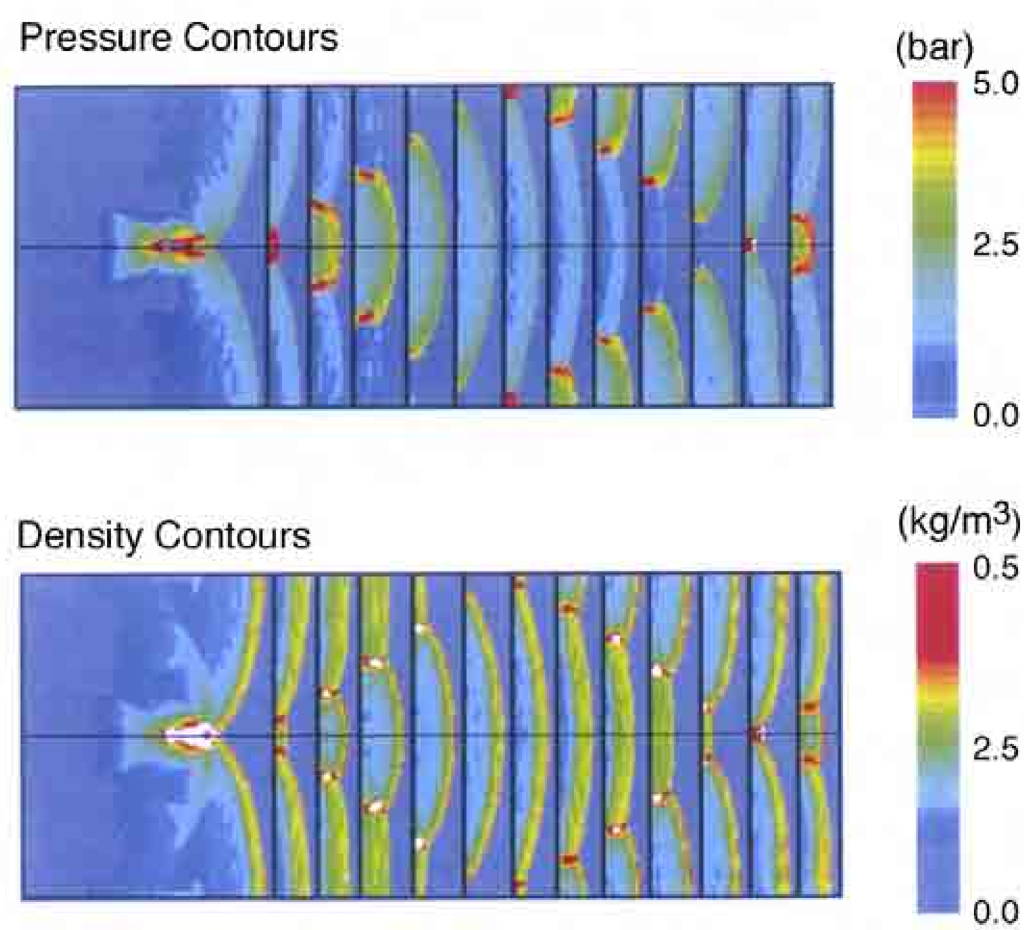
* Multidimensional detonation structure (structure & size)

This is where modern CFD algorithms (FCT, MUSCL, PPM, TVD, etc.) have enabled us to compute accurately enough to be quantitative.

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

.... *Low Pressure*

Detonation cell in a low-pressure (~0.1 atm) H_2-air mixture



Contours shown at ~10 μs intervals.

Contours extracted from simulation every 10 μs **and lined up to show evolving structure of the detonation front.**

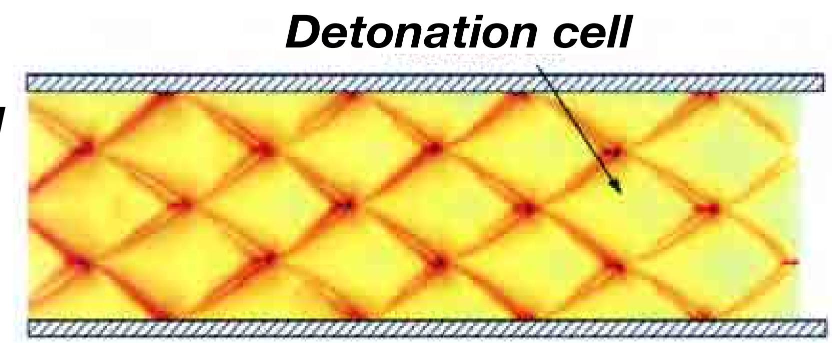
(Oran & Levebvre, 1993)

...... *Low 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.*

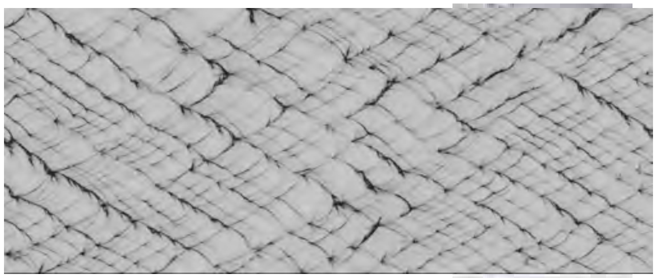
Conclusion: For low-pressure, strong dilution (Ar, N_2) , computed cell sizes are generally within a factor of 2 of measured cell size. Structure looks OK.

Most Recent Detonation Cell Computations

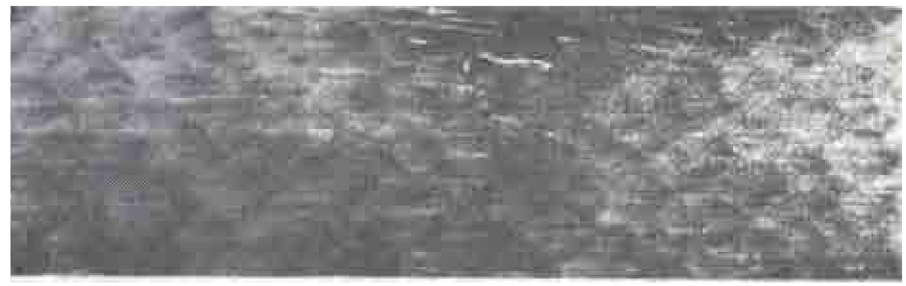
Taylor et al. (2011). H_2-Air, 1 atm, 298K, using mechanism of Burke et al. (with high-pressure correction)

Taylor et al., 2012

4 cm

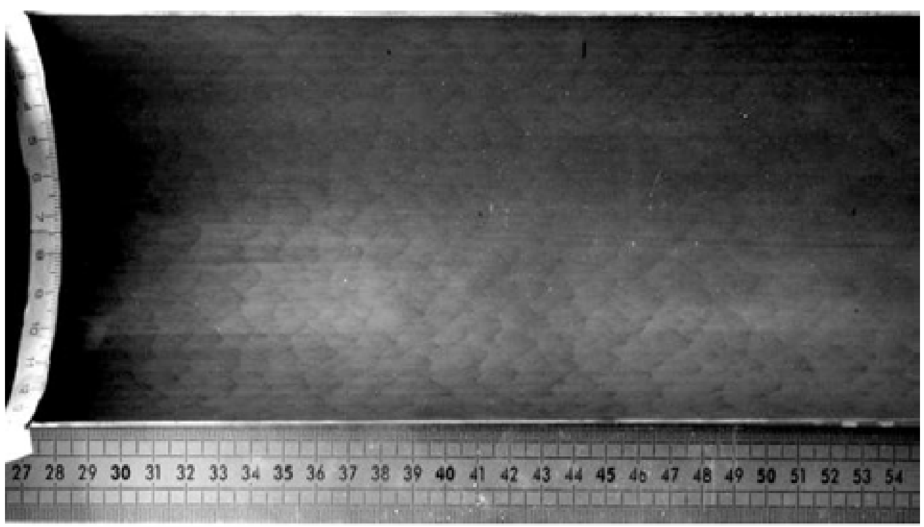


Bull et al., 1982



Poitiers, 2012

12 cm



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.**

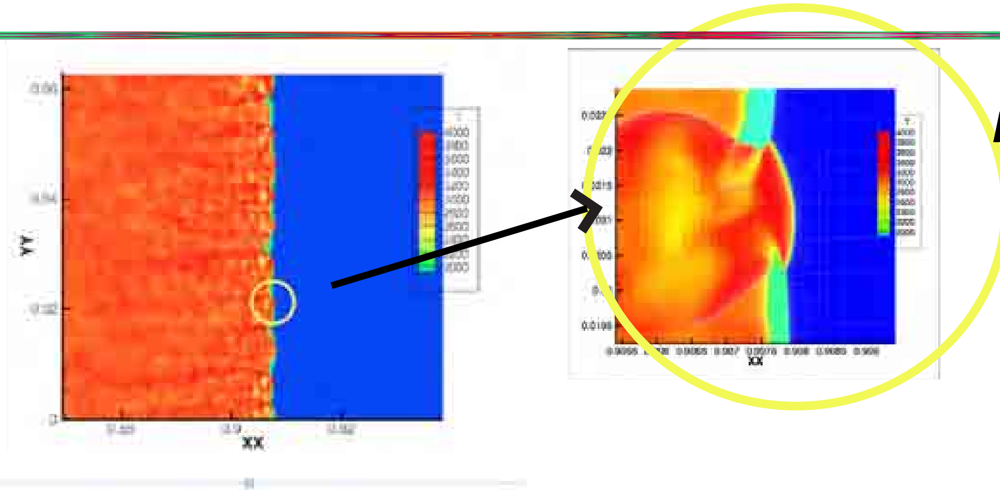
(*Burke et al.* high-pressure chemical model gives cell sizes ~4-5 times too small.)

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

Why???

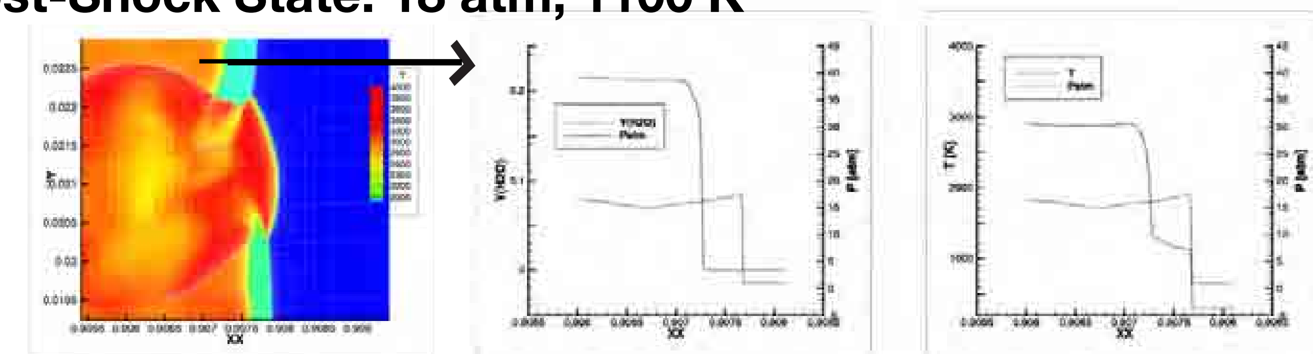
This same trend for computed cell sizes is echoed in measurements and simulations of detonation cells for CH_4-air, 1 atm, 298 K (Kessler et al.).

Reactive Flows under Extreme Conditions

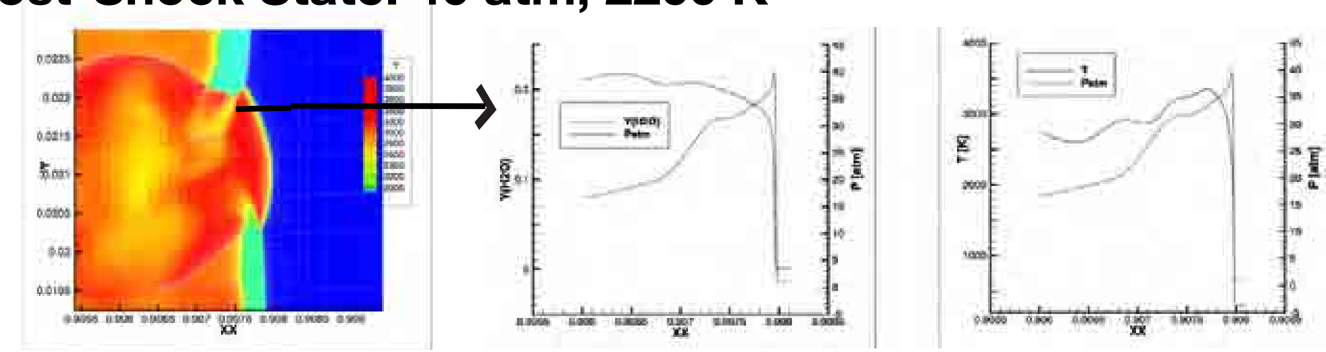


Propagating detonation in H_2-Air, 1 atm, 298K. Burke et al. chemistry. Computations by Taylor, Kessler et al., 2011-12 (Proc.Comb.Inst).

Post-Shock State: 18 atm, 1100 K



Post-Shock State: 40 atm, 2200 K



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

We don't know if the fluid equations hold.
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(And this says nothing about the other terms.)

Lament:

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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."

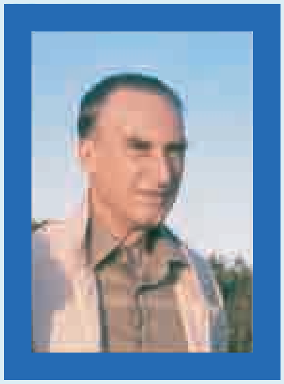
But ...

We don't know what to compute that will make sense,
We don't have input parameters,
We don't know how to model these systems,
We don't know how to connect the right levels of models, even if we have them,

HELP!!!!!

In Memoriam

Huw D. Edwards
University of Wales, Aberystwyth



... an innovative experimentalist with a deep understanding of theory.

Kind, considerate, clever, quick-witted, honest, steadfast -but modest, self-effacing, slow to anger, "a real gentleman" – these are just a few words to paint a ten second profile of Huw's characteristics.

Huw's scientific field was that of gas dynamics and explosions – subjects in which he gained not one but two PhD's, from the Universities of Wales and Cambridge.

His papers are thoughtful, complete meaty treatises noted for the care exercised in obtaining novel experimental data and even more importantly to the time and thought devoted to a careful understanding and analysis. They have stood the test of time - the highest accolade for a scientist's work.

Neither a self-publicist nor a frequent traveler, Huw's way, by and large, was to keep hard at work and mostly in Aberystwyth. But despite this, people from far and wide beat a path to his door - attracted by the topicality and excellence of his work.

The advice Huw gave on careers was "decide what you enjoy doing most in life and get someone to pay you to do it". He should know, because his work was his hobby and his hobby his work.

Adapted from a memorial given by David Bull, November 2003

Founded UKELG (United Kingdom Explosion Liaison Group) in 1981, to link academic research to real world safety problems. UKELG is now planning its 35th meeting.

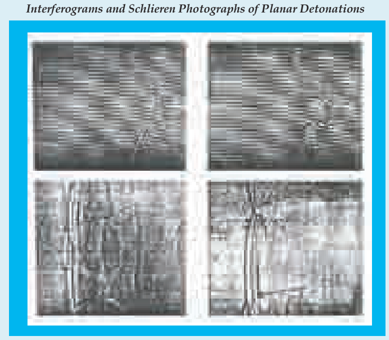
Founding member of ICDERS (International Colloquium on Dynamics of Explosions and Reactive Systems), with A.K. Oppenheim, R. Solukhin, N. Manson, H. Wagner, and R. Strehlow, 1967 in Brussels. ICDERS is planning its 20th biennial meeting.

Through his work with the Ministry of Defense, he helped shape the policy of the Health and Safety Executive in Great Britain

Pioneering Development and Application of Diagnostic Techniques for Shocks and Detonations include:

Development of piezo-electric pressure bar gauge, the Edwards guage (1958)
Application of mercury discharge lamp to Schlieren photography (J. Sci. Instru., 1957)
Development of microwave techniques for:
Velocity measurements of marginal detonation waves (J. Phys., 1970)
Ionization measurement in reactive shock and detonations (J. Phys., 1971)
Study of unstable detonations (J. Phys., 1974)
Continuous measurement of velocity of galloping detonation waves
Pressure and velocity measurements of detonation waves (JFM, 1959)
Temperature measurements from relative emission intensities of OH ultraviolet bands (J. Phys., 1974)

Interferograms and Schlieren Photographs of Planar Detonations



Elucidation of Detonation Physics

Oblique shock waves in detonations (JFM, 1963)
Structure of wave front in spinning detonation (JFM, 1966)
Induction zone studies of detonation waves (Trans. Faraday Soc., 1967)
Reflected shock interaction process in a shock tube (AIAA J, 1968)
Structure of transverse waves in detonations (Astro. Acta, 1969)
Strength of transverse waves in marginal detonation waves (J. Phys., 1971)
Location of C-J Surface in a multiheaded detonation wave (J. Phys., 1976)
Simulation (experimental) of detonation cell kinematics using 2D reactive blast waves (J. Phys., 1983)
Coupling spinning detonation and oscillations behind wave (J. Appl. Phys, 1966)
Longitudinal instabilities in detonation waves (C&F, 1971)
Instabilities in reaction zones of detonation waves (Astro. Acta, 1972)
Instabilities near limits of propagation (J. Phys., 1977)
Direct Initiation of spherical detonations (Astro. Acta, 1976)
Quasi-steady regime in critically initiated detonation waves (J. Phys., 1978)
Detonation initiation by planar incident shock-waves (C&F, 1981)
Effects of tube diameter in gaseous detonations (Nature, 1957)
Collapse of transient cavities in water (JFM, 1960)
Detonation diffraction at an abrupt area change (JFM, 1979)
Cavitation experiments using a water shock-tube (J. Phys., 1980)
Shock diffraction in channels with 90-degree bends (JFM, 1983)
Gas dynamics of vented explosions (C&F, 1985)
Detonation quenching by water sprays (CST, 1990)
Detonation behavior at concentration gradients (C&F, 1991)
Detonation in porous structures (Prog. Astro. Aero, 1991)

Unreacted Pockets behind Detonations

Shock-to-Detonation Transition

Thank you for your kind attention !