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Triton Fun Company Science Newsletter April 2009

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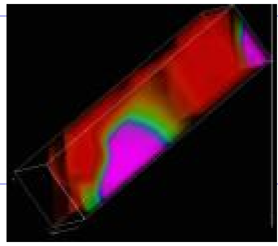
Detonation Physics: How it all works



S. Kao

Special points of interest:

- Shock physics
- Triton Fun stuff
- Superfluous questions

We are always looking for **contributors** to the Science Newsletter. If you would like to write an article about a science subject you are excited about, or contribute a superfluous question, or if you would like to be on our **mailing list** for future newsletters, please e-mail us at:

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We have all seen TV shows and movies depict the detonation of high explosive. While their special effects are fun to watch and impressive, the scientific definition of a detonation is much more specific. A *detonation* is a *supersonic combustion wave in which a shock wave and a reaction zone are coupled*. Basically, a shock wave moves through a chemical mixture causing reactions as it goes through and generates a moving *transition zone* where the chemistry is taking place. The leading shock raises the temperature and pressure of a mixture of fuel and oxidizer initiating a coupled thermal branching-chain explosion. After an induction time, exothermic (heat-generating) recombination reactions create product species whose expansion acts as a piston propelling the shock wave forward. The interaction between the leading shock wave and consequent reaction zone is a defining characteristic of self-sustained detonations.

Further, experiments and numerical simulations of detonation propagation problems are also characterized by unsteady motion due to the intrinsic instability of the reaction zone structure. This instability may arise due to the sensitivity of the reaction rates to temperature fluctuations. The temperature varies over very short spatial scales in the transition zone and the sharp gradients accelerate reactions.

Arrhenius proposed in 1889 that the reaction rate depends on temperature in the following way: $k = A \exp(-E/(RT))$. From this, we see that small fluctuations in the leading shock speed which are manifested as small changes in the temperature lead to large changes in the reaction rate. While this is the most commonly discussed cause for the instability, several other mechanisms have been proposed.

The focus of my thesis work was the underlying physics and chemistry of this apparent instability. I used a very simplified chemistry model and the compressible inviscid fluid equations of motion to study the fundamental characteristics of gaseous detonations. We found that even the most simple, realistic systems are too complicated to model with much accuracy. It has always amazed me that even though man has had fire for thousands of years, we still do not understand the process of combustion very well. In fact, even with today's computing power, we still cannot simulate all the elements of a seemingly simple candle flame.

An interest in detonation instability arose in the 1960's when experimental results showed that detonations were inherently unstable. White first observed in 1961 this instability using a technique called *interferometry*. At the same time, Denisov and Troshin (1959) and Shchelkin and Troshin (1965) used the popular *soot foil* technique (described below) to record histories of the detonation instability. The results of these experiments indicated that detonations were complex *three-dimensional phenomena* with *nonplanar shock fronts* and *turbulent reaction zones*.

Based on research of detonations, we know that this instability is somewhat periodic and varies with chemical mixture. This prompted researchers to investigate the character of the instability and important parameters governing the behavior. The "soot-foil" technique involves putting a thin layer of soot on a piece of aluminum and then putting the aluminum along the wall of the detonation tube. As the detonation runs over the soot, it will leave behind a diamond pattern in the soot particle which defines its "cellular structure". Some mixtures, i.e. those highly diluted with argon, exhibit "regular" cellular structure where all of the diamond shaped cells are roughly the same size and shape.

continued, pg 2 —>

Explosive physics: *continued*

Photos/Info: Univ. of Illinois/LANL/D.S.Stewart/T.D. Aslam/Univ of Leeds/G.J. Sharpe/Yokohama National Univ/K. Ishii/Air Force Inst of Tech/GDT

On the other hand, mixtures diluted with nitrogen will exhibit "irregular" cellular structure. Irregular structure can simply mean cells of varying shape and size as well as double cellular structure where each large cell is filled with smaller cells. Currently, our group is working to characterize the chemistry behind this double cellular structure.

An example of a system where detonation would be occurring would be, for example, the complete combustion of propane. In its reaction with oxygen to form water and carbon dioxide, the vapor pressure of the products is higher than the reactants and so the additional pressure increases the effect of the shock wave as it goes through the medium, multiplying the reaction.

In an effort to investigate the most influential parameters on combustion, researchers investigated the linear stages of detonation instability. Strehlow et al (1967) seem to be the only researchers successful at visualizing the onset of instabilities experimentally, but many researchers, including myself, have studied it numerically. It appears that the effective activation energy of the reaction system, i.e. the activation energy of a fictitious global reaction describing the system, is a critical parameter.

Although the work I did is still very idealistic and not yet entirely of practical use in the real world, I hope it will pave the way for more of a bridge between experiment and computation throughout the field of combustion.

I enjoyed my research because I was able to take a natural phenomenon that is extremely complex and fascinating and express a facet of it in tangible mathematical terms. Next time you watch a movie or TV show where some type of high explosive is detonated, think about the physics and chemistry that allow it to happen and how cool the instability makes it look.

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References:

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Shchelkin, K.I., and Y.K. Troshin, *Gasdynamics of combustion*, Mono Book Corp., Baltimore, MD (1965)

Strehlow, R.A., R. Liaugminas, R.H. Watson and J.R. Eyman, Transverse wave structure in detonations, Proc. 11th Intl Symposium on Combustion (1967)

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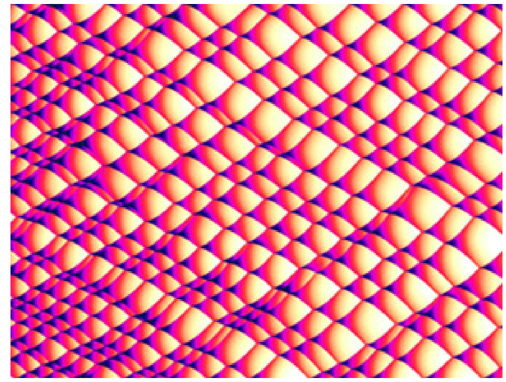
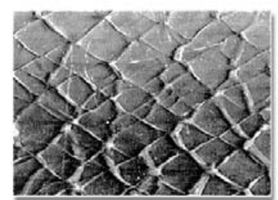
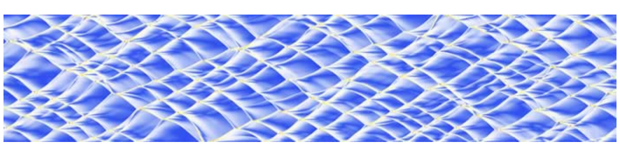


Computation and simulation of the "cellular" pattern generated by a **detonation shock wave front** in a soot foil experiment
(Univ. Illinois/LANL)

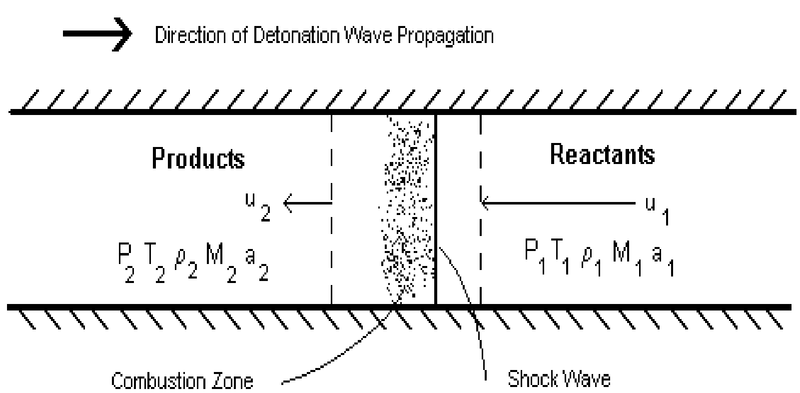


Soot-foil test on $H_2 + O_2$
Cellular structure on a smoked foil after passing through of a detonation wave (Yokohama U)

Detonation wave propagation showing movement of shock wave and combustion zone. As the shock wave propagates through the chemical constituents, reactants are converted to products via combustion
(Air Force Inst of Technology/A.J. Rolling thesis)



Numerical simulation of cellular dynamic of detonation waves. The cellular structure comes from parts of the wave moving through at different angles at different times.
(Univ of Leeds)



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2009 has been declared the "International Year of Astronomy". Events and activities to further the excitement of astronomy are being planned by IYA committees in over 100 countries. The logo for the IYA2009 is shown below. For more info on upcoming IYA2009 events, go to: http://www.astronomy2009.org

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Superfluous Questions:

1) Bylot Island is part of *what* country ?

   a) Russia b) Norway c) Canada d) Japan

2) The Azores are an island group residing in what ocean ?

   a) Pacific Ocean b) Arctic Ocean c) Indian Ocean d) Atlantic Ocean

3) What island contains the wettest spot on Earth (i.e., gets the most rain) ?

   a) Madagascar b) Galapagos c) Kaua'i d) Skye

4) Which island is the smallest island nation ?

   a) Barbados b) Fiji c) Nauru d) Iwo Jima

—> ANSWERS in next months issue of the Science Newsletter ! <——-

** ANSWERS to March's Superfluous Questions: 1. c) Baranov 2. d) Miscellaneous Affairs 3. c) Frost Building 4. c) Billy