Numerical Simulations of Reactive Flows – Subsonic to Hypersonic, Millimeters to Kilometers

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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,...

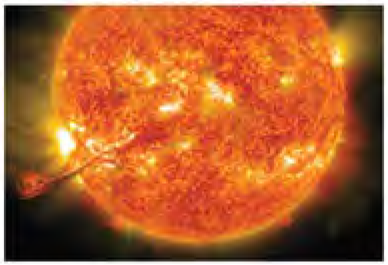
Despite the obvious physical differences among these flows, there is a striking similarity in the forms of the descriptive equations. Thus the considerations and procedures for constructing numerical models of these systems are also similar."

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

Reacting flows of curent importance, consisting of flames or detonations, chemical or nuclear, confined or unconfined, single or multiphase, generally turbulent, and so on ... .

Local flow speeds range from subsonic to supersonic, over ranges from meters to kilometers

Coronal Magnetic Eruption 2012

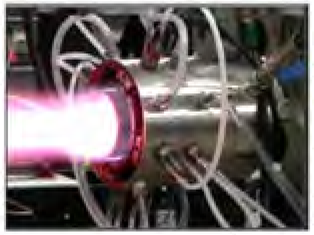


Wildfires ... Colorado 2012

Aircraft explosion 2008

Mine Explosion Greymouth

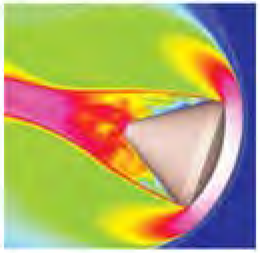
Rotating Detonation Wave Engine



Annulus perpendicular to inlet and nozzle. Incoming propellents are continuously ignited, and detonate, producing thrust.

(Courtesy UT Arlington)

Atmospheric Reentry Flow



Scramjet Engine

Pulse Detonation Engine

... and usually under highly stressed, nonequilibrium conditions.

Issues for Numerical Simulations

Flow speeds range from very slow (subsonic) to very fast (supersonic, hypersonic?) in one simulation, perhaps in different locations simultaneously.

Complexity - must represent many physics processes,
need information from many technical fields.

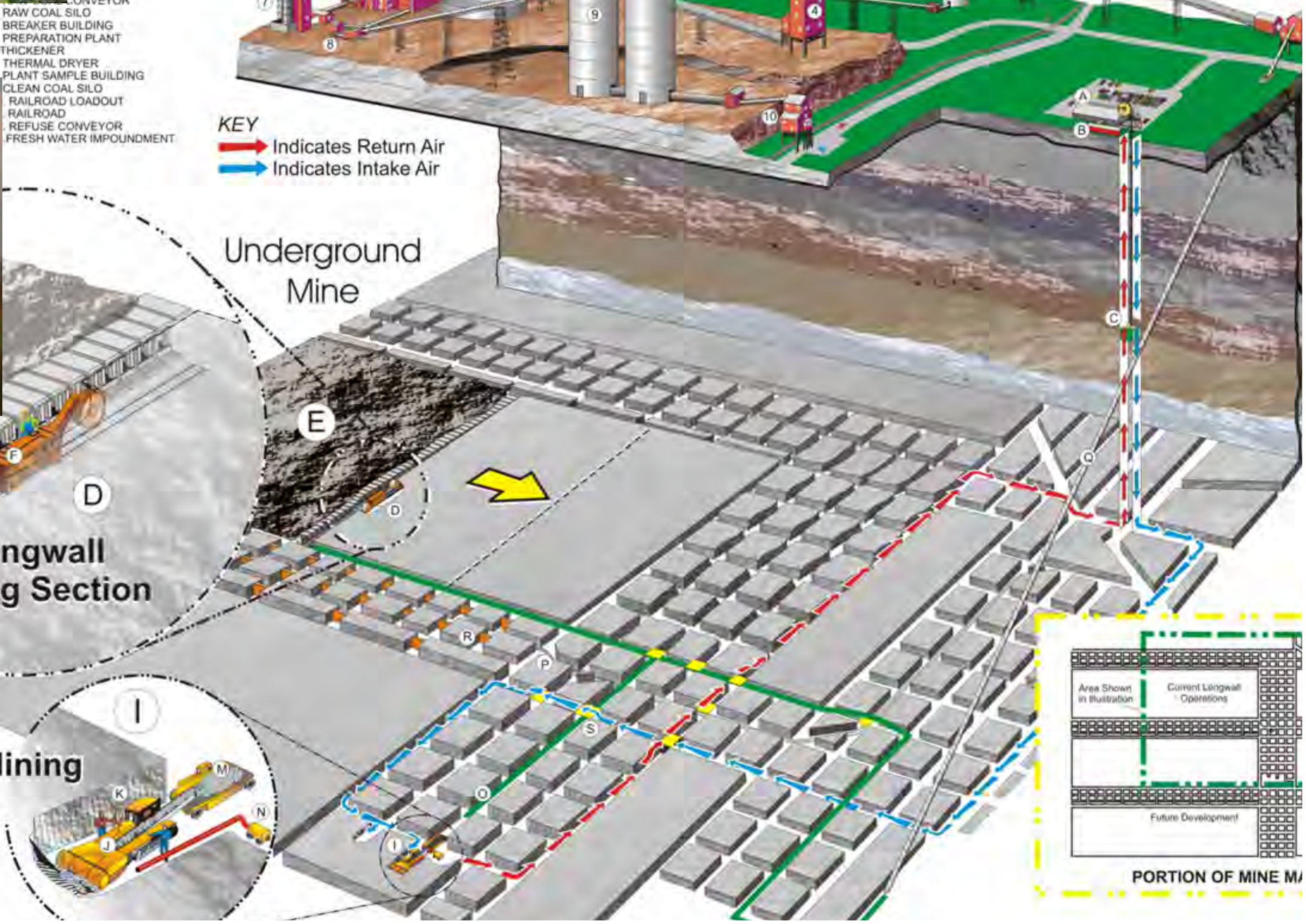
Range of relevant scales can be for
Terrestrial problems of interest:
spatial resolution: 5-6 orders of magnitude,
velocity of features: ~4 orders of magnitude
temporal range: 6-7 orders of magnitude
Astrophysical problems, possibly much wider range.
Implication for the selection of algorithms and methods.

Computer resources -- processors, memory, computer time, diagnostics, data transmission, ...

Schematic of a Coal Mine

Greymouth

Radspadskaya



Natural gas seeps in from walls.

A Natural Gas Explosion in a Coal Mines

These are the basic questions asked by NIOSH and other agencies and foundations:

Given a large enough volume of a flammable mixture of natural gas and air, such as may exist in a coal mine, can a weak flame or spark ignition develop into the most powerful form of reaction wave, a detonation?

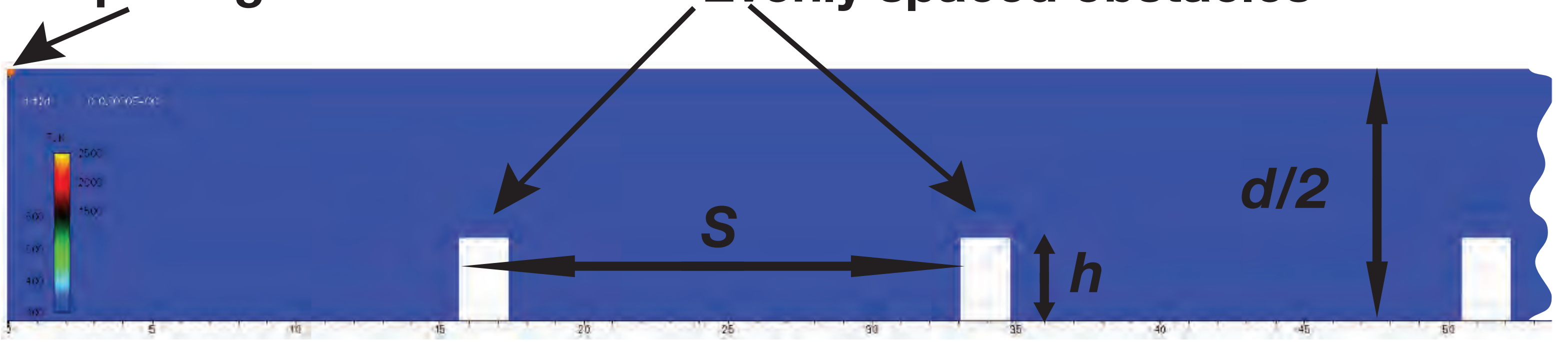
Led to work funded by NIOSH, the Alpha Foundation for Mining Safety, and others interested in natural gas.

Detonations generate considerably higher pressures than turbulent flames ...If CH_4 detonates, does it create pressures on separation barriers exceeding regulations?

This is a question of general theoretical interest with immediate practical concerns.

Natural Gas (CH_4) and Air

Simulations Proposed



Spark ignition

Evenly spaced obstacles

S

h

$d/2$

(cm)

Experiments Proposed : channel 1 m diameter

Existing previously

Tube diameters:

d = 17.4, 52, 10 cm

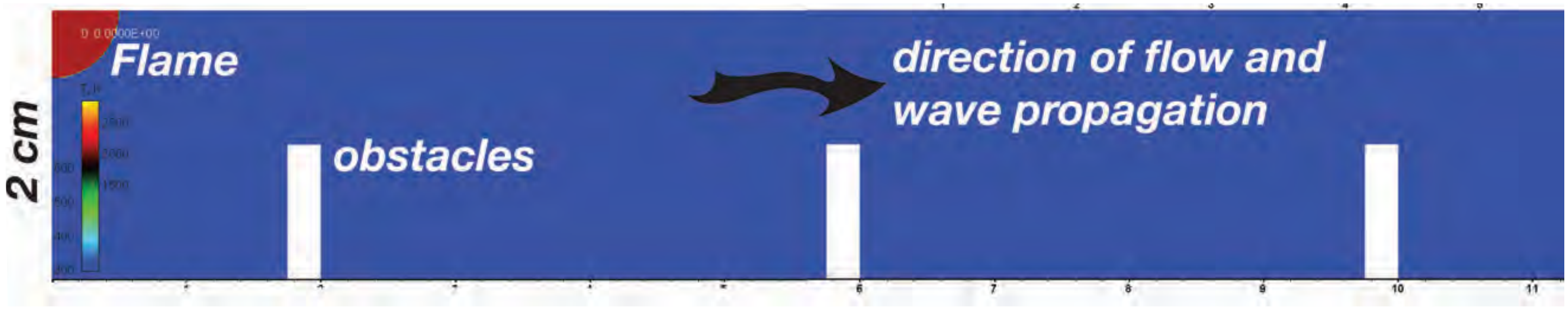
Blockage ratios:

h/d = 0.3, 0.6

Cylindrical tube

At that point, we had already shown how DDT can happen in a channel with obstacles ...

Consider a hydrogen-air mixture in a channel.
Initially, there is a small flame in top corner.

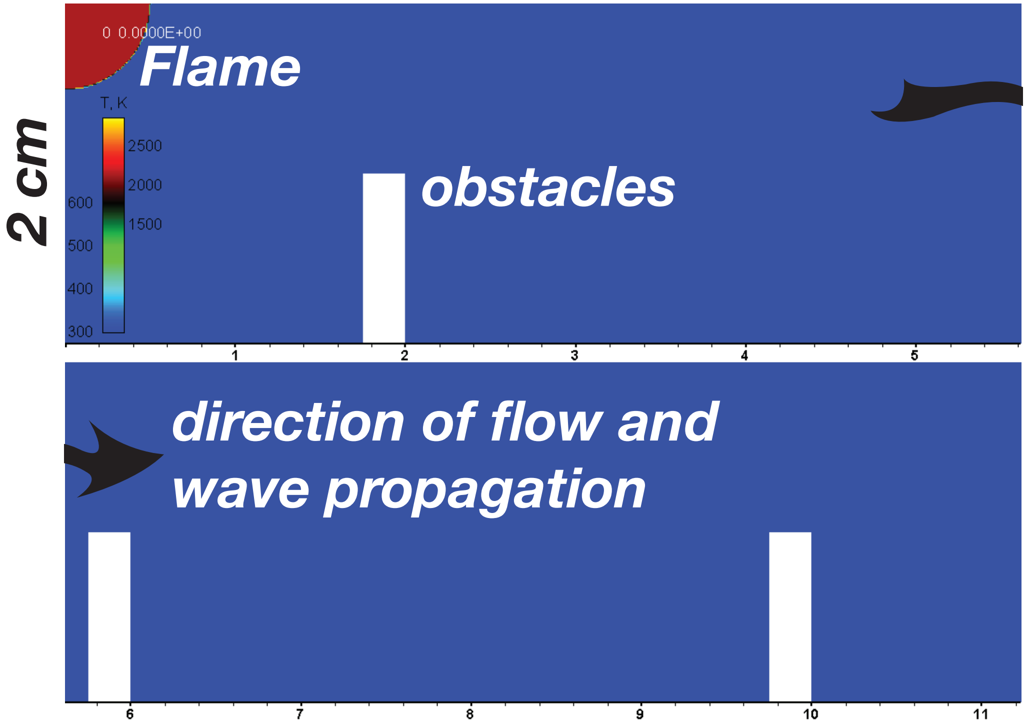


This computation was done for Japanese NEDO project to look at safety issues in hydrogen refueling stations.

The results of this hydrogen study was really a breakthrough in our understanding DDT in confined, obstructed spaces.

Numerical Simulations of a 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 flame develops and produces shock waves. This leads to the formation of unsteady shock-flame complexes and detonations.

What the Movie Showed Us ...

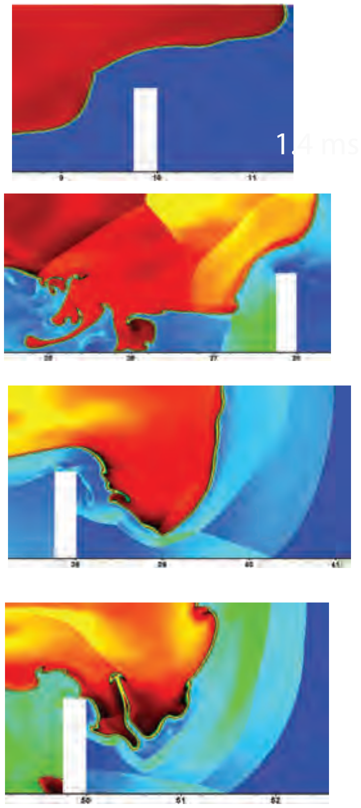
The initially laminar flame moves slowly into unreacted material.

Obstacles perturb the flow. Flow interacts with and distorts the flame. The flame accelerates and becomes turbulent.

The turbulent flame generates compression waves, which eventually coalesce to form a shock in front of the flame.

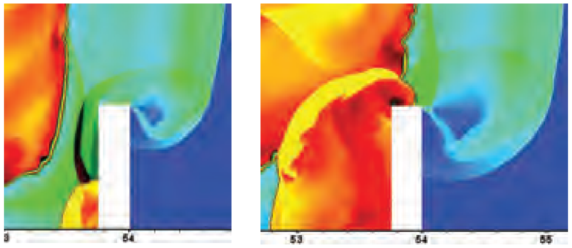
The shock is continuously strengthened by compression waves coming from behind.

Temperature Contours



A shock-flame complex forms (fast flame).

Shocks reflects from obstacles, create *hot spots,* or *ignition centers,* ignition centers, that may become spontaneous waves.



Simulation requires resolution down to flame thickness, millimeters. System height is centimeters, the length meters.

Numerical Solution Approach to Reactive Flows

Solve the unsteady, compressible Navier-Stokes equations in one-, two-, and and three-dimensions by five (!) different numerical methods: **low-order Gudonov (Gamezo), high-order FCT (Ogawa), high-order PPM (Poludnenko), high-order Gudonov (Ogawa), and most recently high-order WENO (Houim).**

Include submodels for chemical reactions, energy release, thermal conduction, molecular diffusion, etc., and *calibrate them to reproduce basic flame and detonation properties*.

Resolve the flow down to necessary microscale (viscous, other?)

-- direct numerial simulation (DNS), or

-- AMR (adaptive mesh refinement) by fully *threaded tree* (FTT) or *block refinement (PARAMESH)*, BoxLib, or AMRex

Simulate specific laboratory experiments, some specifically designed to test the model. Experiments on DDT (Thomas et al.), on hydrogen flame acceleration (Teordorczyk et al.), and natural gas, (Kuznetzov et al., and Zipf et al.).

Numerical Solution Approach to Reactive Flows

Solve the unsteady, compressible Navier-Stokes equations

Any monotone method, of reasonable order, is adequate for the problem.

Include submodels for chemical reactions, energy release,

Input usually not clearly known;
Solution very sensitive to this.

Resolve the flow down to necessary microscale (viscous, other?)

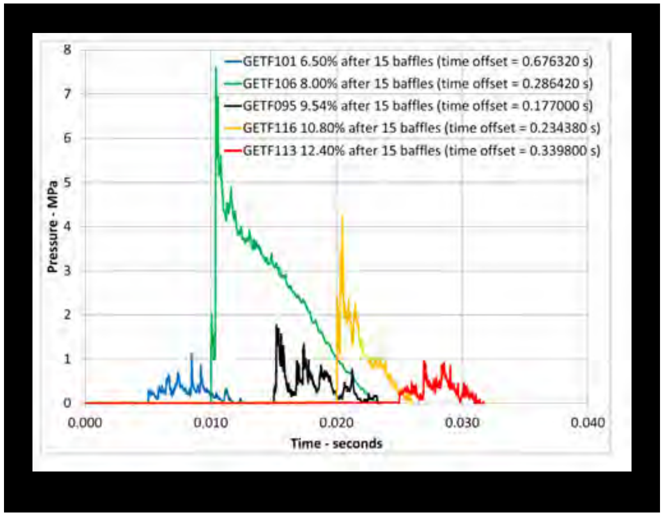
There is a minimum resolution for largest and smalled computational cell size. This requires care and testing. Dynamic adaption is important.

Simulate specific laboratory experiments

... when these are available. Don’t expect absolute agreement.

Some of the Results of Experiments and Simulations

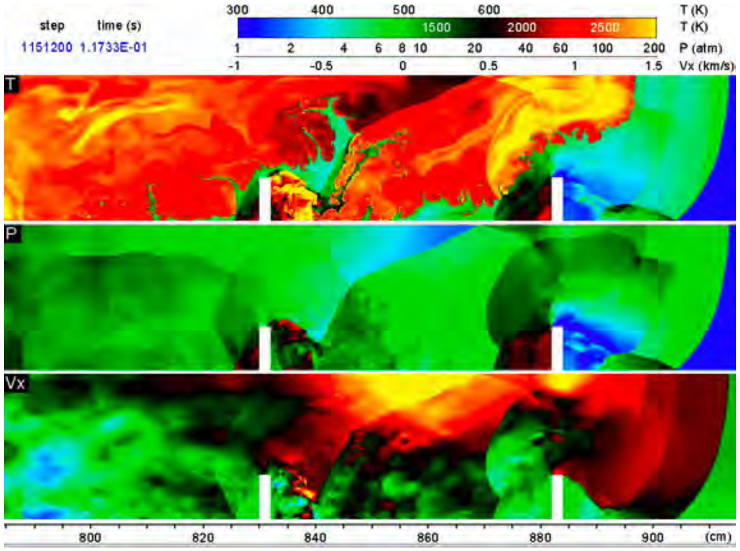
The Experiments:



" ... DDT within the baffled section of the tube and sustained detonations beyond the baffles in the smooth part of the tube were observed over the composition range 8.0 to 10.8% NG-air."

(Zipf et al, CNF 2014)

The Simulations –
How it all works ... .

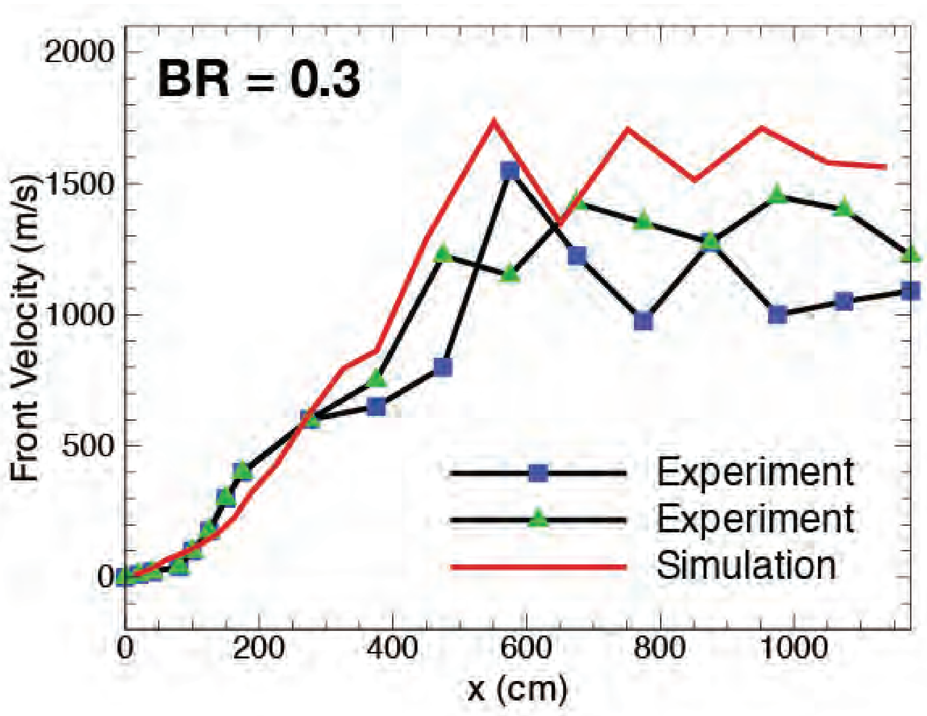


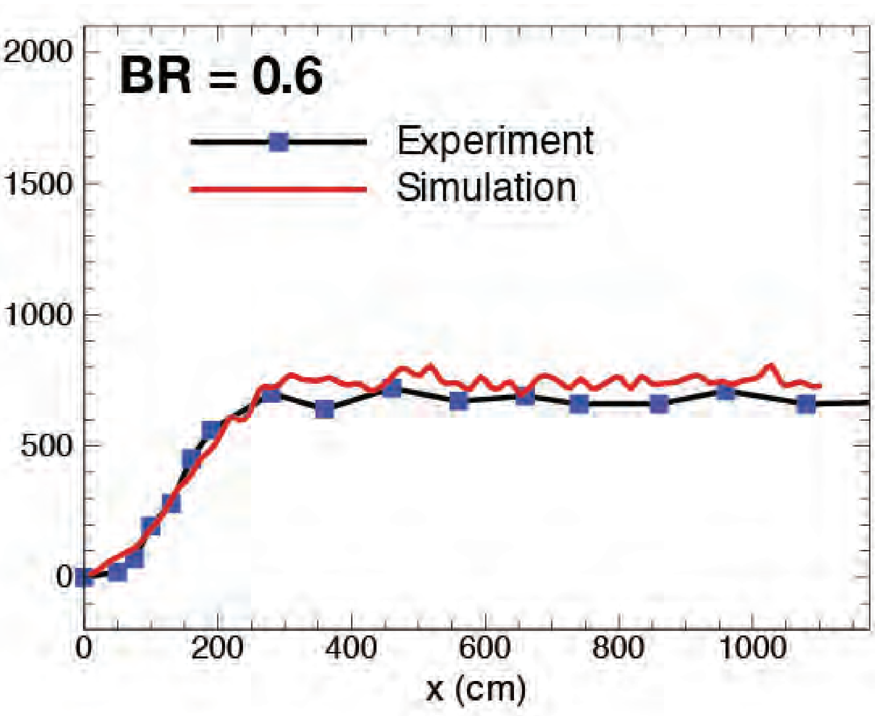
(Kessler, Gamezo et al,)

Lorem ip

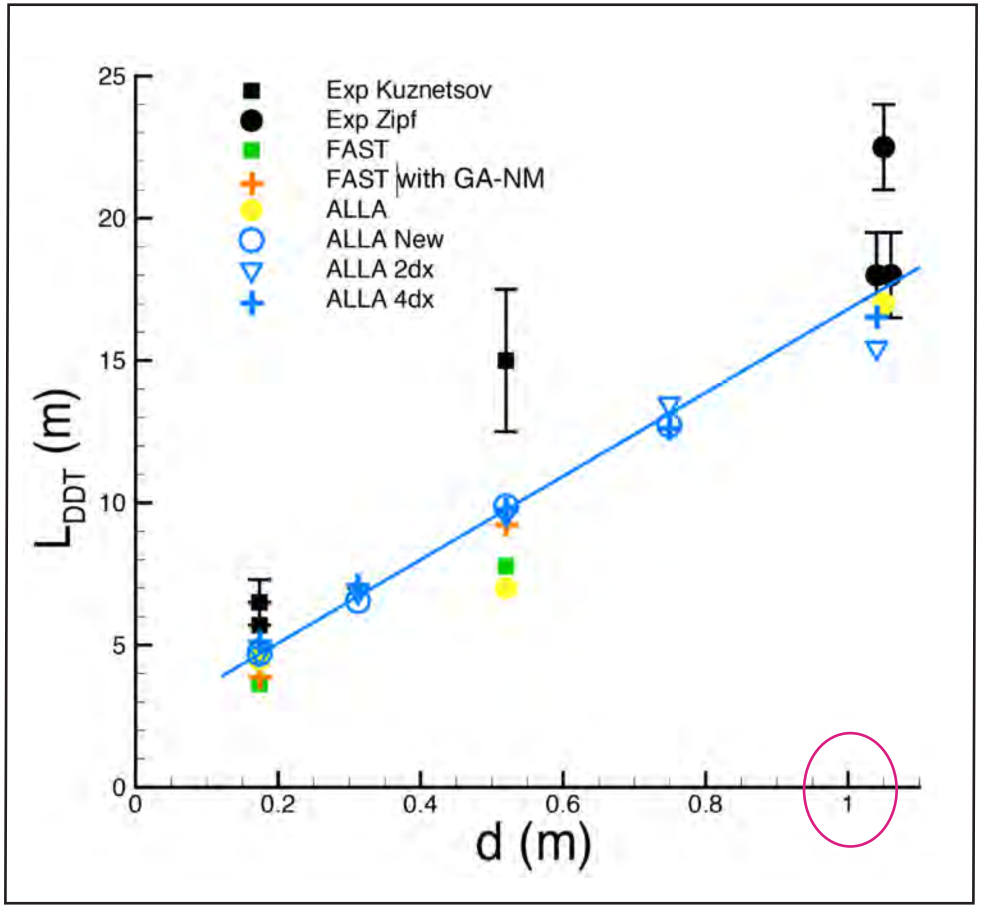
Movie Shows:

Acceleration of the initial flame
Formation of a turbulent flame
Formation of shocks
Interactions among shocks, flames, boundary layers
Formation of hot spots (gradients of reactivity)
Hot spots “decay” to shocks and flames
Hot spots transition to detonations





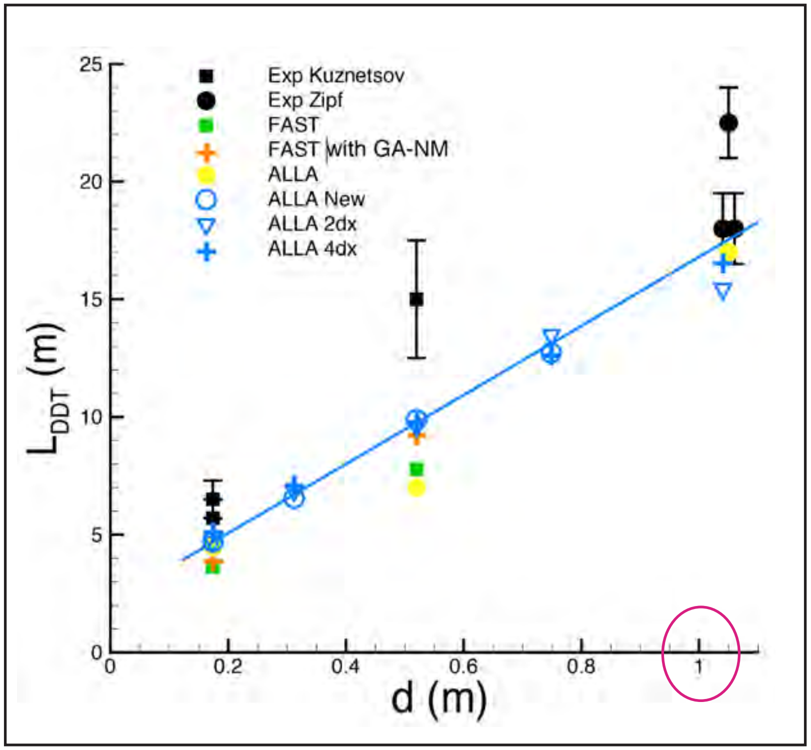
Scaling Law and Approach to Larger Systems



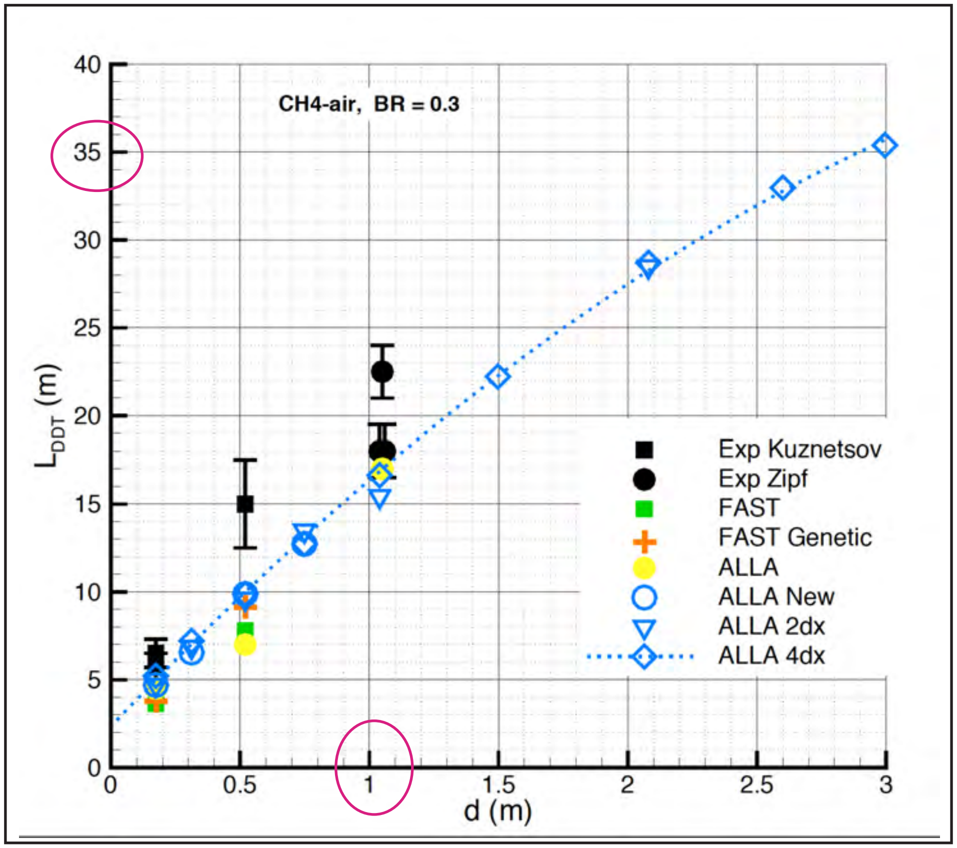
Fix blockage ratio, and space between obstacles, vary channel height.

Benchmark lower-order code (ALLA) again the higher order code (FAST).
Learn how to use (and trust) ALLA for simulations of larger systems.

Note the change in the scaling as system size increases.



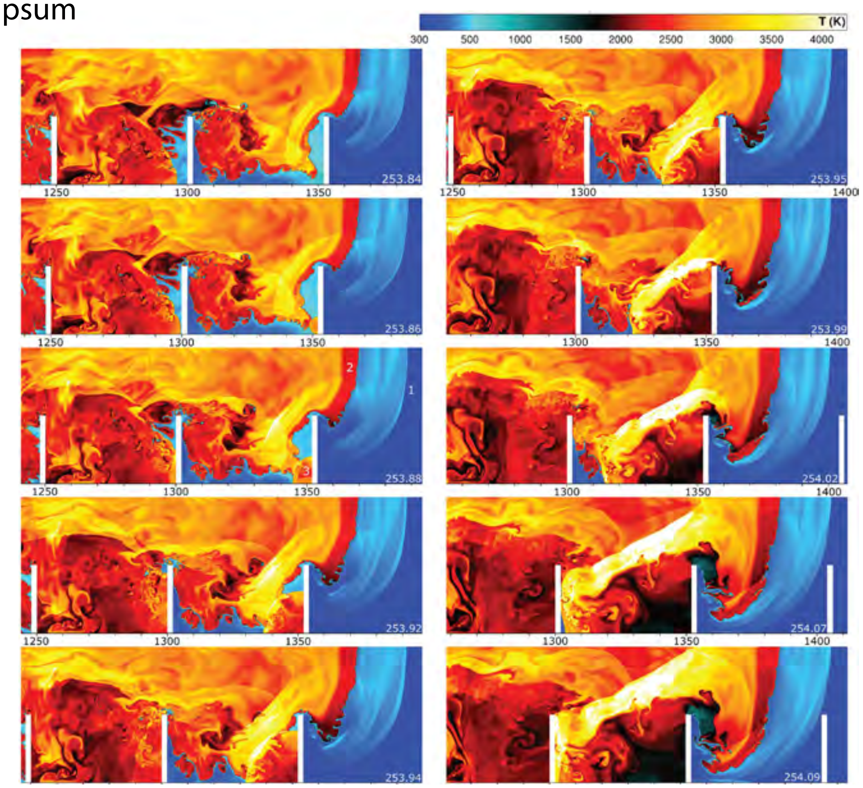
Curve is no longer linear for larger systems.



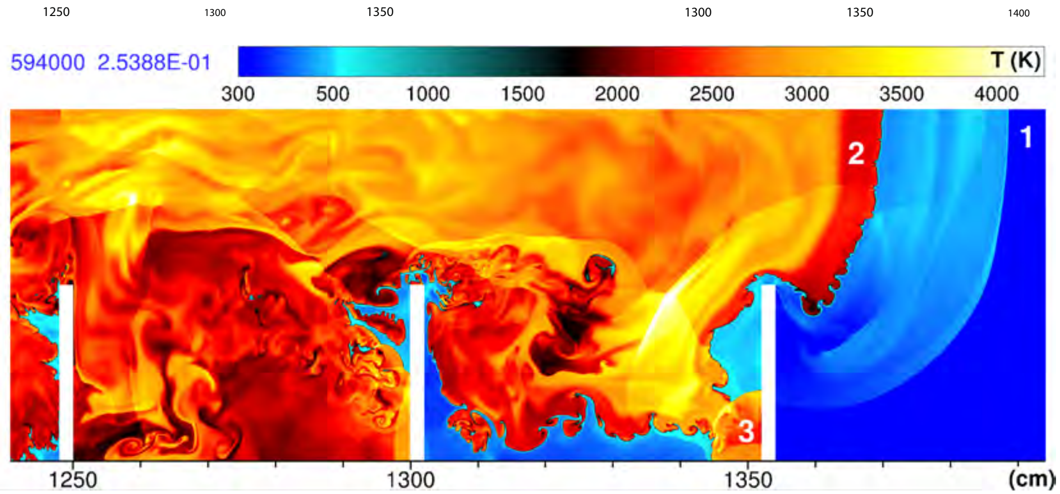
Other physical effects become important.
(E.g., 3D turbulence?
More time for boundary layers to develop between obstacles?)
More experimental data might help resolve this!

Three-Meter High Simulation

Lorem ipsum



This particular run required ~95 hours on 128 cores (32 cores/node) of a computer using Intel Xeon Skylake 6130 processors in 2019 (uninterrupted for data dumps for movies).



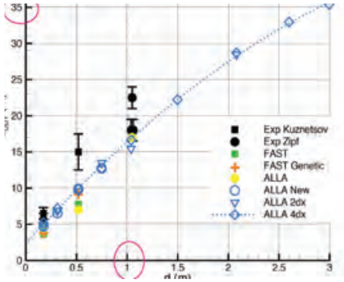
Conclusions and Discussion

1. *Simulations have shown that natural gas can detonate in configurations that are on the scale of coal mines (3 m height).*

2. *Experiments and simulations have shown that it is easier to detonate natural gas in larger than smaller systems. (That is, it can be detonated for leaner mixtures.)*

3. *Simulations that predict scaling laws for distance-to-detonation (in obstacle-laden flows) in natural gas indicate that a change in importance of physical processes for larger size systems. (Note turn-over of the curve.)*

Is this an effect of changes in character of turbulence, distance from walls, accuracy of model, etc? Requires experimental verification.



4. *For all of the channel sizes studied, the mechanism leading to detonation was essentially the same: the formation of a turbulent flame, a shock-flame complex, and then a Mach stem reflection from an obstacle that ignited a detonation.*

Conclusions and Discussion

What we need now …

One or two extremely resolved 3D simulations of one of the larger systems.

This would answer several of the remaining physics questions with respect to the importance ofr turbulence and boundaries.

Simulations of direct ignition, from a flame or spark, no obstacles

This would determine if we can predict absolute detonabiity at the lean detonation limits.

So far, this only can be done experimentally.

Collaborators in this Program

Vadim Gamezo – US Naval Research Laboratory
Takanobu Ogawa – Seikei University

Karl Zipf – Consultant, NIOSH (retired)
David Kessler – US Naval Research Laboratory

Ryan Houim – University of Florida
Huahua Xiao – USTC (Hefei, China)
Gabriel Goodwin – US Naval Research Laboratory
Alp Ozgen – Kale Arge, Istanbul

Carolyn Kaplan – University of Maryland

Logan Kunka – Texas A&M University
Xiaoyi Lu – Texas A&M University

Thank you for your kind attention !