Computational Flame Propagation Studies in Support of Launch Vehicle Risk Assessment

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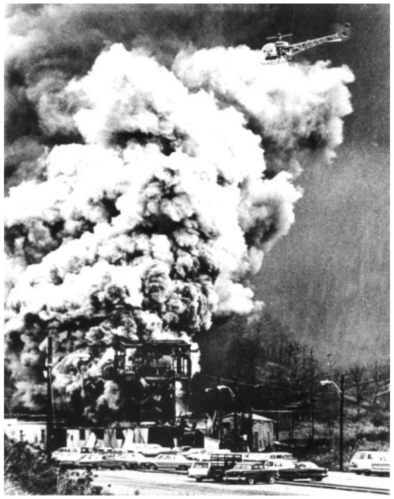
PhD Dissertation Work
Stanford University

Motivation

Antares Rocket
Turbopump failure, Fire in leaking fuel
Lost payload



Texas City Refinery
Hydrocarbon vapor cloud explosion
15 people killed

Farmington Mine
Presumed methane gas explosion
78 people killed

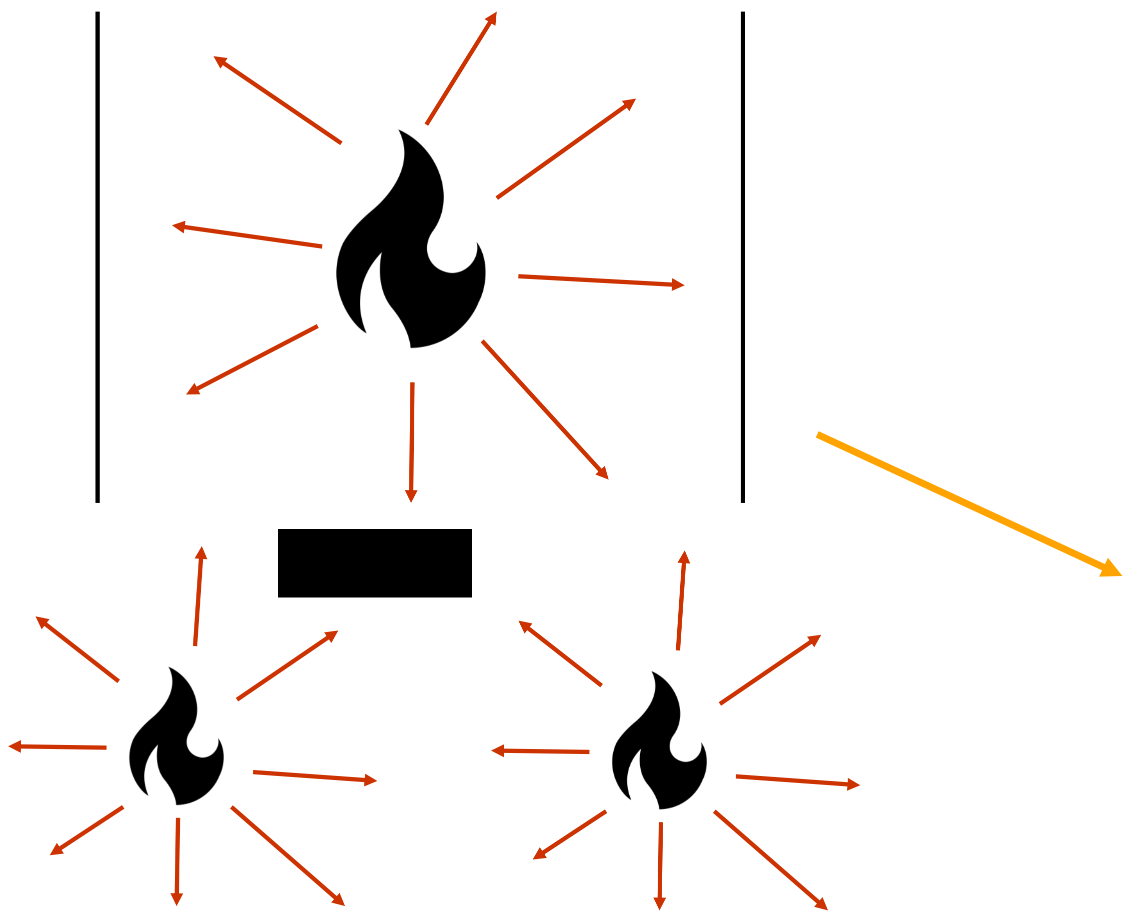
http://www.csb.gov/assets/news/image/BP_PLANT_EXPLOSION-1_lowres2.jpg https://www.flickr.com/photos/nasahqphoto/15470323057/ http://www.msha.gov/TRAINING/LIBRARY/historyofminerescue/page6.asp#.UyotHKhdUdU

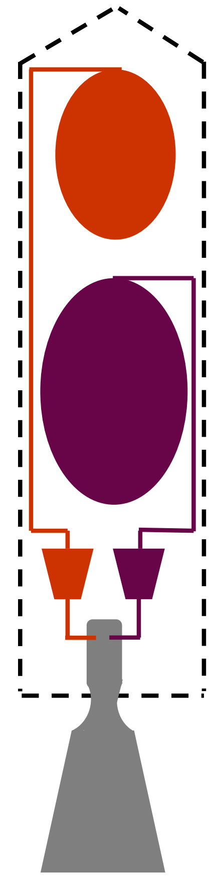
Motivation

Low ignition energy makes hydrogen dangerous

Static Spark

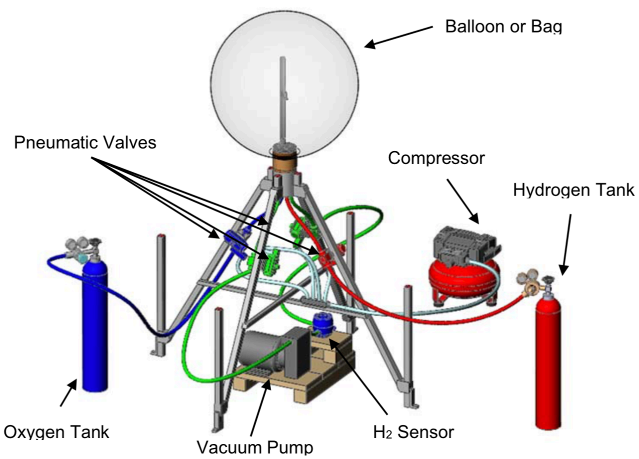
Motivation



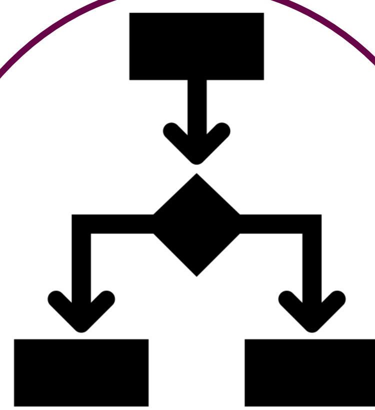


Motivation

Blast environments for these events are difficult to characterize



Experiments



Engineering-level Blast Model

CFD Simulations

E. Richardson, T. Skinner, J. Blackwood, M. Hays, M. Bangham, and A. Jackson. An experimental study of unconfined hydrogen/oxygen and hydrogen/air explosions. 46th Joint Army-Navy-NASA-Air Force (JANNAF) Combustion Conference, 2014.

https://images.nasa.gov/details-ARC-2008-ACD08-0272-002

Motivation

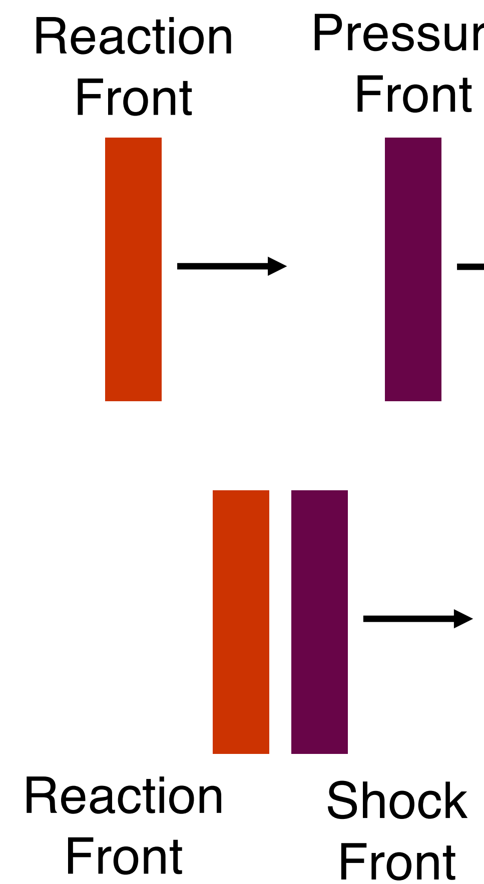
Deflagration: Subsonic (relative to surrounding gas) flame propagation driven by heat transfer

Detonation: Supersonic (relative to surrounding gas) flame propagation with a shock directly ahead of the flame

DDT: Deflagration to detonation transition

Overpressure: Pressure above ambient pressure

Deflagration $P/P_0 \approx 1.1 - 2$
Detonation $P/P_0 \approx 25$



Research Outline

Understand flame propagation mechanisms and sensitivities through the use of computational simulations to inform risk assessments which lead to safety guidelines and influence the design of safer vehicles

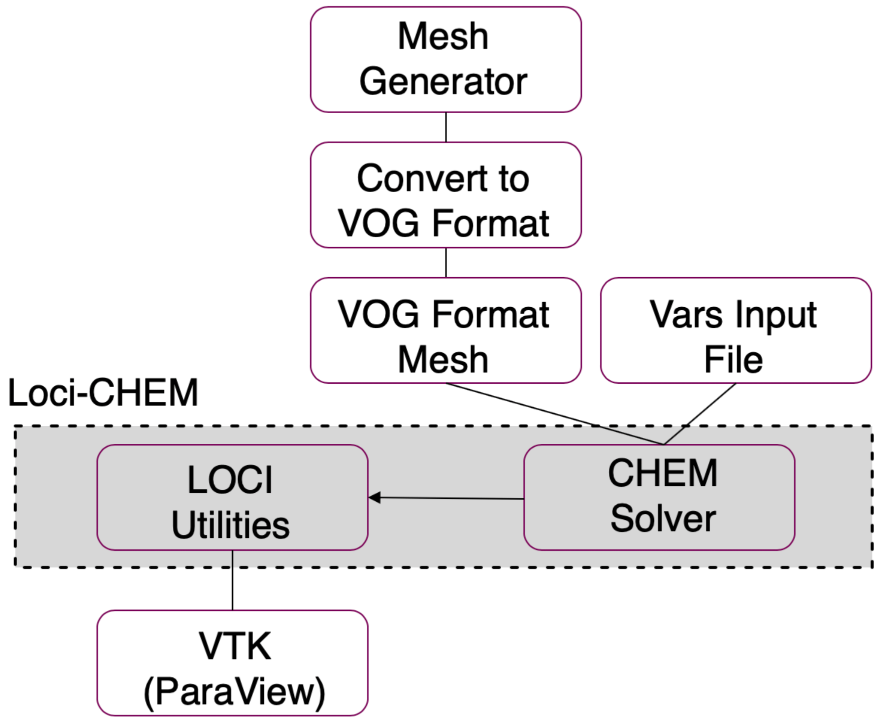
Mechanisms of deflagration to detonation transition (DDT) in confined, obstructed flows

Influence of underlying flow parameters on propagation and comparisons to experimental data and engineering model results

General Approach

- Loci-Chem CFD Code
  - Density-based, finite volume, unstructured solver
  - 2^{nd} order accuracy time and space
  - Navier-Stokes in three dimensions
  - Viscous, turbulent, chemically reacting flows

- Solver
  - Symmetric Gauss-Seidel solver
  - MUSCL scheme for finite volume method
  - Barth flux limiter



General Approach

- Models
  - Built-in database for transport and diffusion models
  - Menter's Baseline turbulence model
  - 7-species, 8-reaction H_2-O_2 chemistry model

Arrhenius Form

$k=AT^B\exp(-C/T)$

- Mesh
  - Ideally several points within laminar flame thickness, order of 0.3 mm
  - Grid spacing on the order of 0.1 mm – up to 4 orders of magnitude smaller than domain
  - Assume axisymmetric geometries, 2D meshes

Reactions

1	$H_2 + M \rightarrow H + H + M$
2	$O_2 + M \rightarrow O + O + M$
3	$H_2O + M \rightarrow OH + H + M$
4	$OH + M \rightarrow O + H + M$
5	$H_2O + O \rightarrow OH + OH$
6	$H_2O + H \rightarrow OH + H_2$
7	$O_2 + H \rightarrow OH + O$
8	$H_2 + O \rightarrow OH + H$

Forward Rate Constants

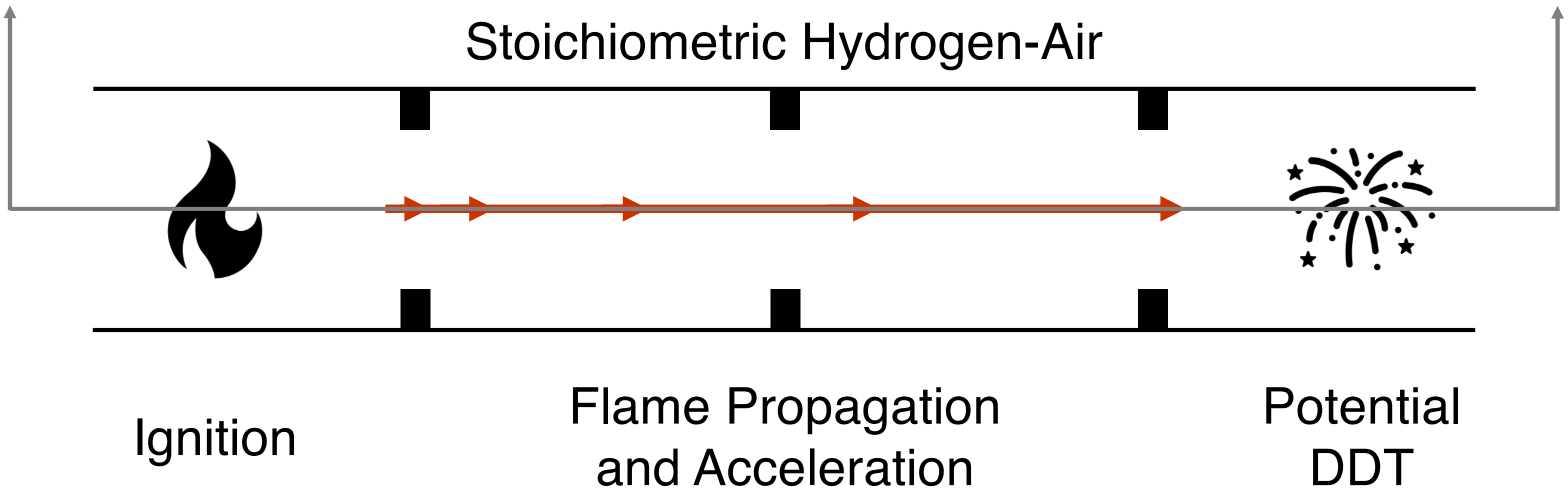
	A	B	C
1	5.5×10^{18}	-1.0	51987
2	7.2×10^{18}	-1.0	59340
3	5.2×10^{21}	-1.5	59386
4	8.5×10^{18}	-1.0	50830
5	5.8×10^{13}	0	9059
6	8.4×10^{13}	0	10116
7	2.2×10^{14}	0	8455
8	7.5×10^{13}	0	5586

J.S. Evans and C.J. Schexnayder. Influence of chemical kinetics and unmixedness on burning in supersonic hydrogen flames. AIAA Journal, 18:188–193, 1980.

TRANSITION TO DETONATION WITH OBSTACLES IN THE FLOW

A.M. Coates, D.L. Mathias, and B.J. Cantwell. Numerical investigation of the effect of obstacle shape on deflagration to detonation transition in a hydrogen–air mixture. Combustion and Flame, 209:278–290, 2019.

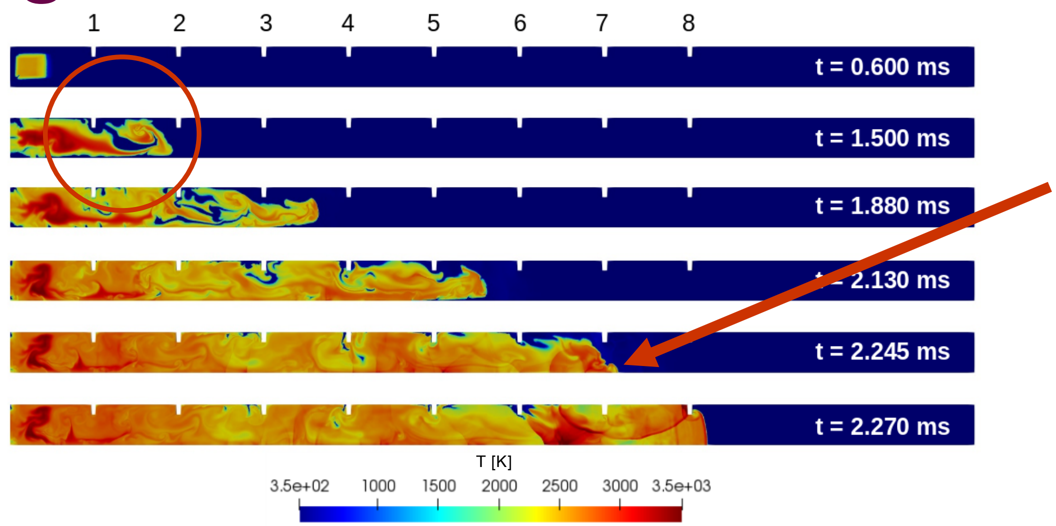
Introduction



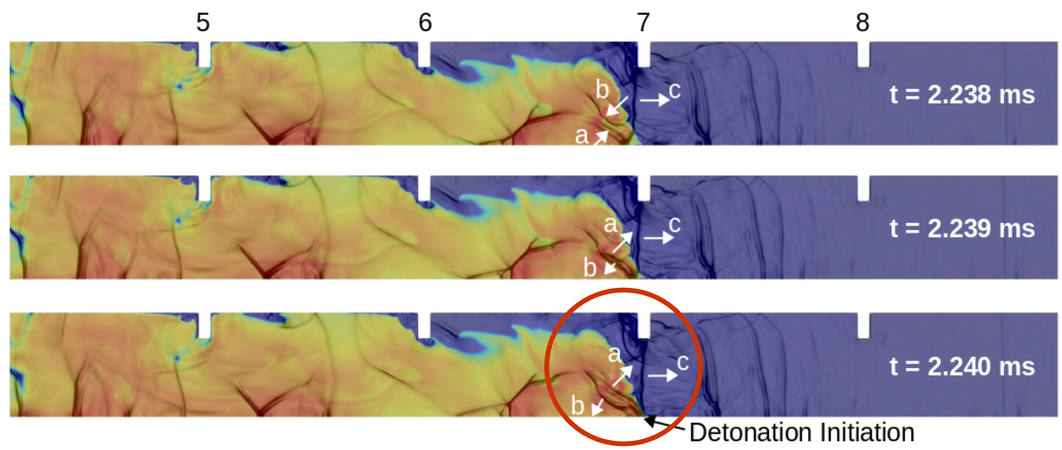
- Obstacle shape
- Number of obstacles
- Ignition source
- Initial conditions

Rectangular Obstacles

Temperature contours

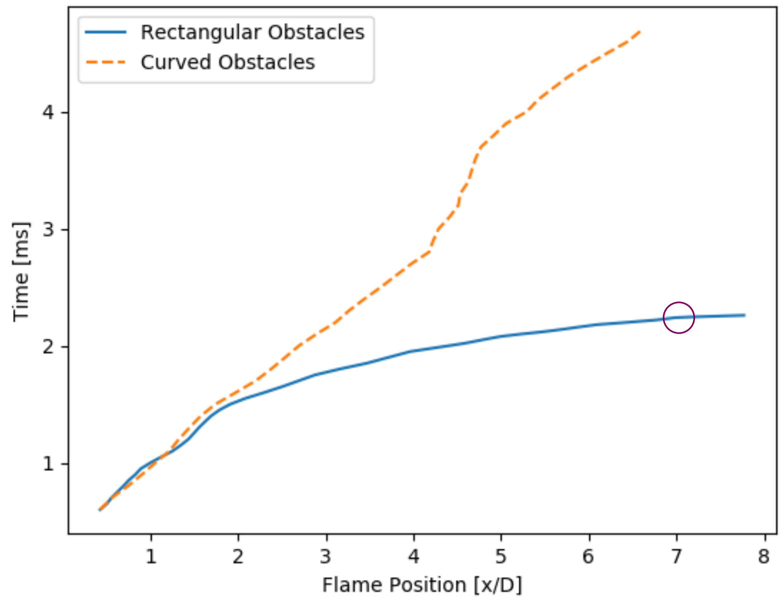


Temperature contours
Pressure gradient overlay



Curved Obstacles

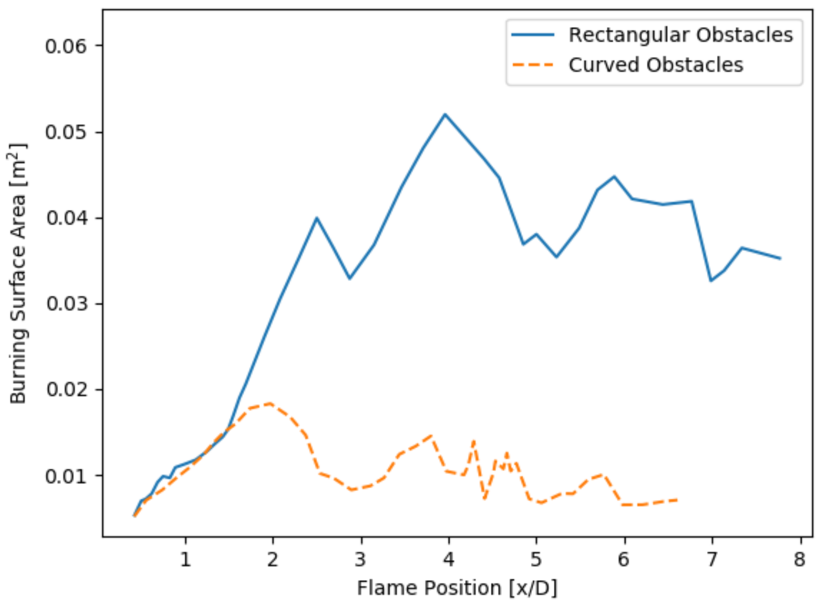
- Reduces recirculation behind obstacles and reflections off the front of obstacles



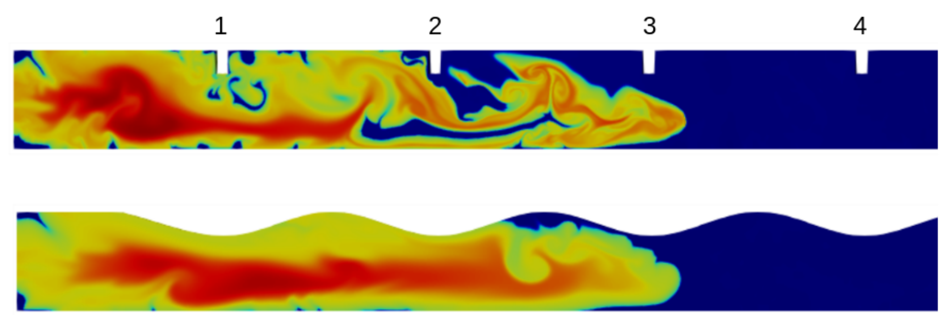
No Detonation

Detonation

Curved Obstacles

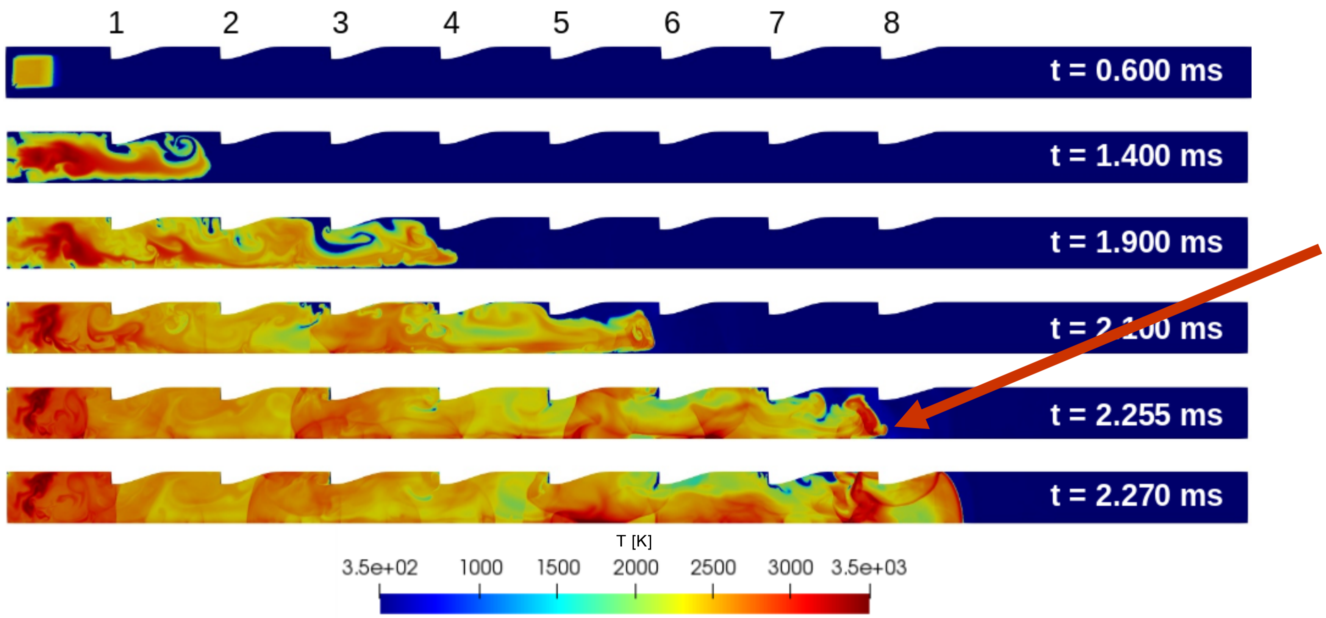


Burning Surface Area → Flame Acceleration



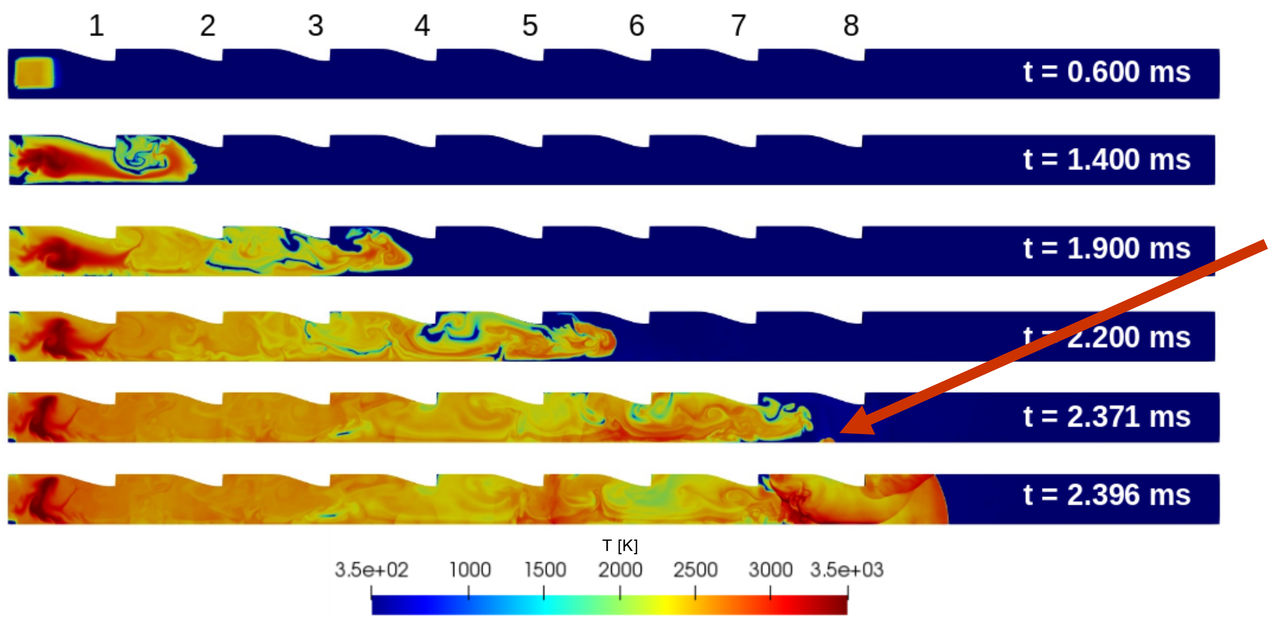
Aft Curved Obstacles

- Maintain forward pressure reflections while reducing aft mixing



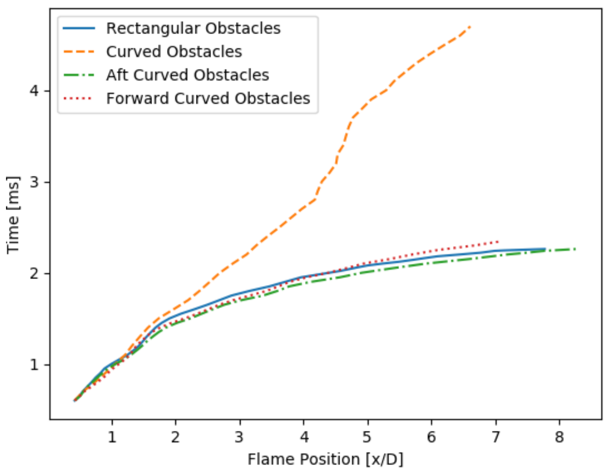
Forward Curved Obstacles

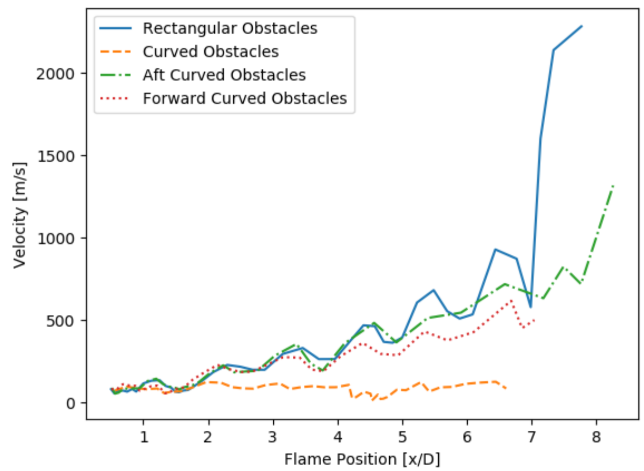
- Limit forward pressure reflections while maintaining aft separation and mixing

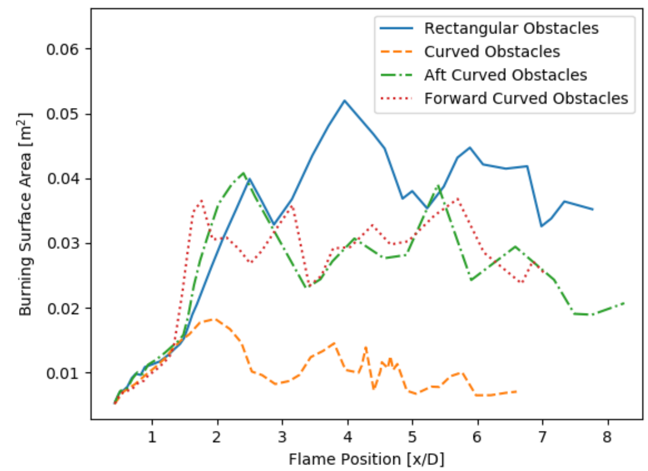


Compare Obstacle Shapes

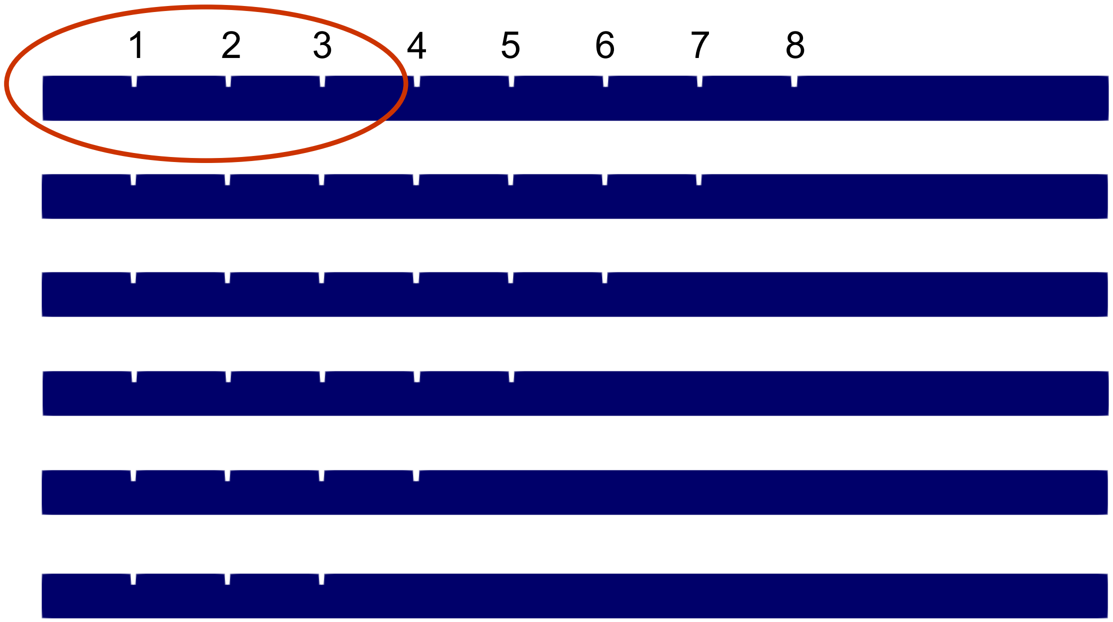
Sharp Edge Obstacle → Aft Separation, Vortical Regions → Increased Burning Area → Flame Acceleration → DDT

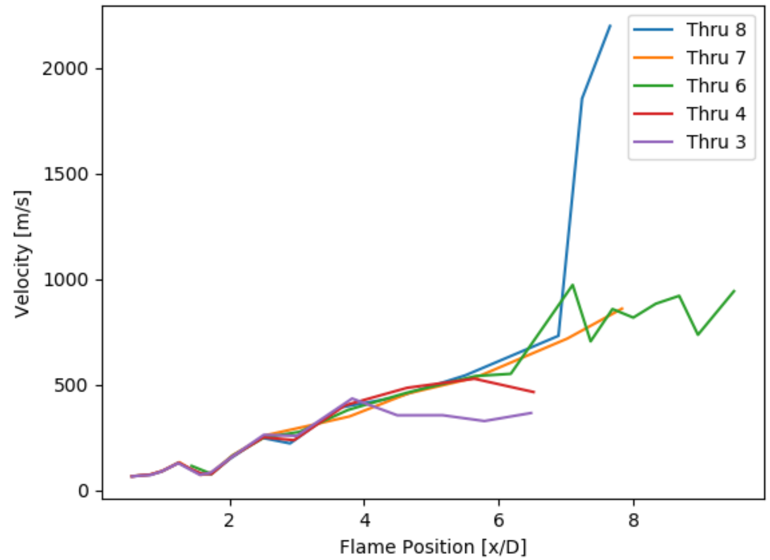


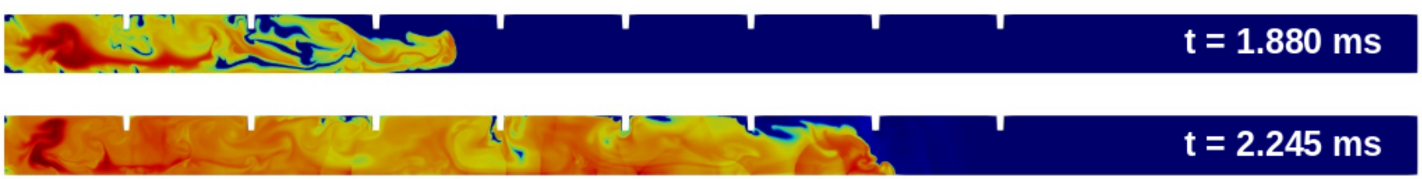




Obstacle Number Variation

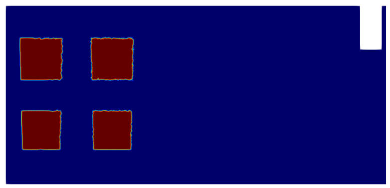






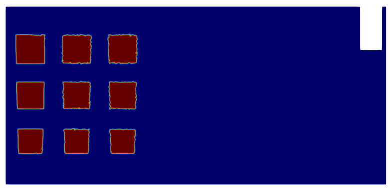
Ignition Source Variation

1 source



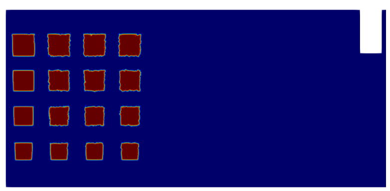
4 source

2 source (Horizontal)

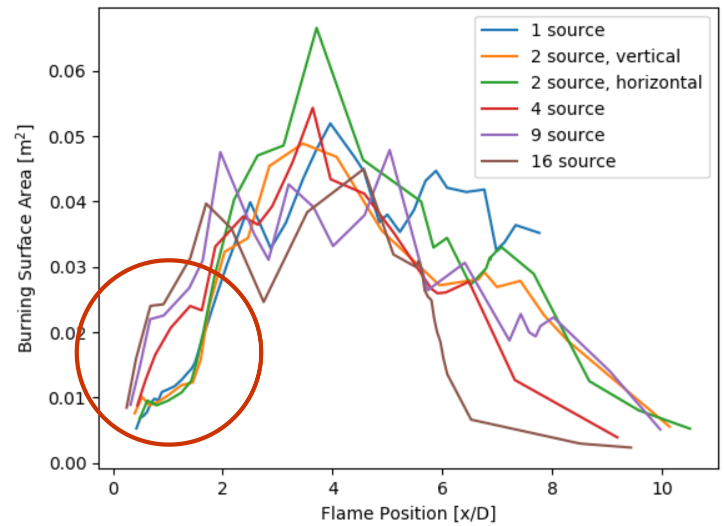


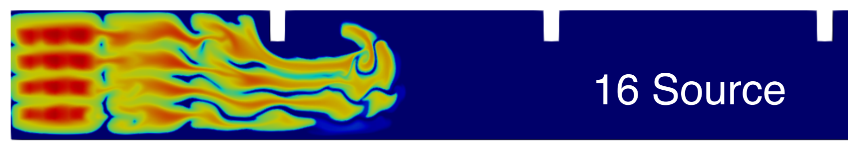
9 source

2 source (Vertical)



16 source

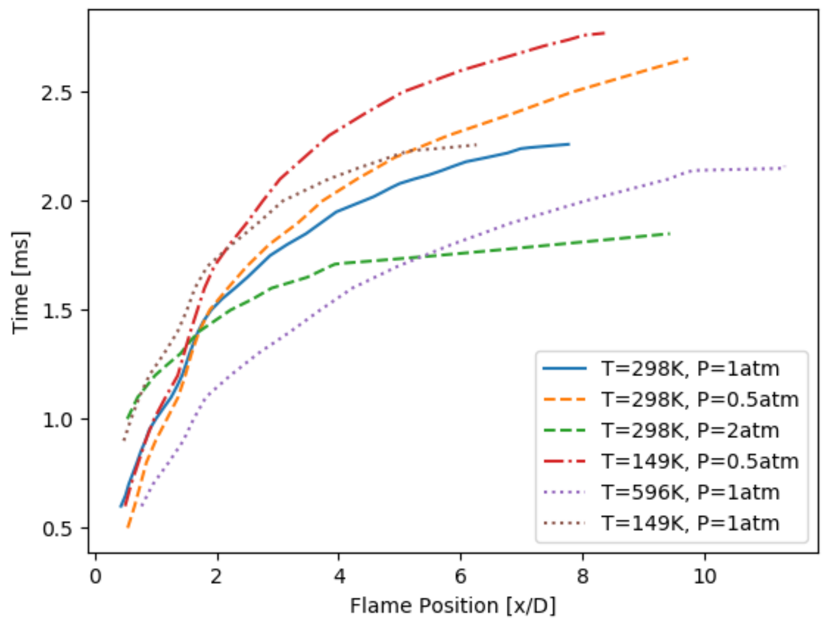


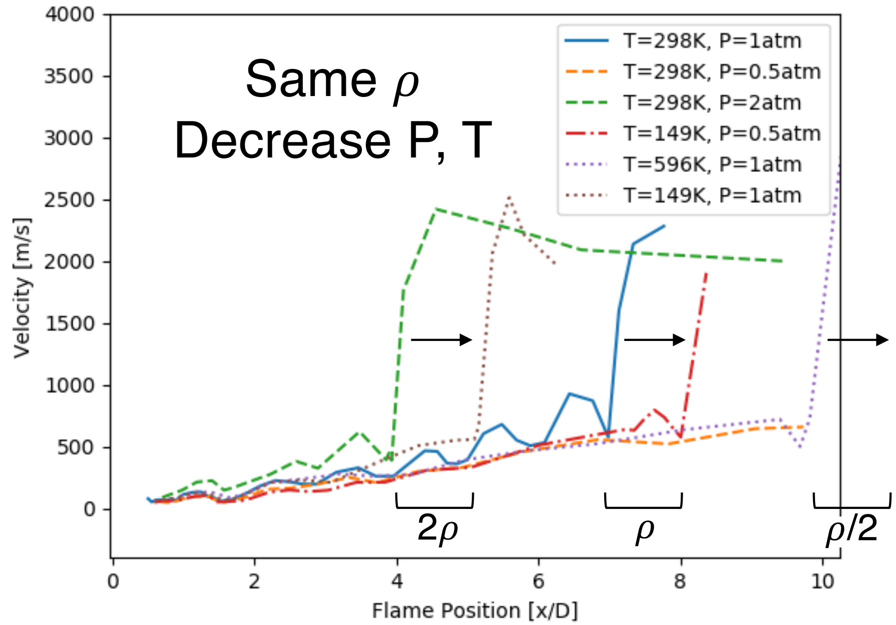


Reduced time to DDT by 25%

Initial Condition Variation

- Considered pressure (P), temperature (T), and density (ρ) variations





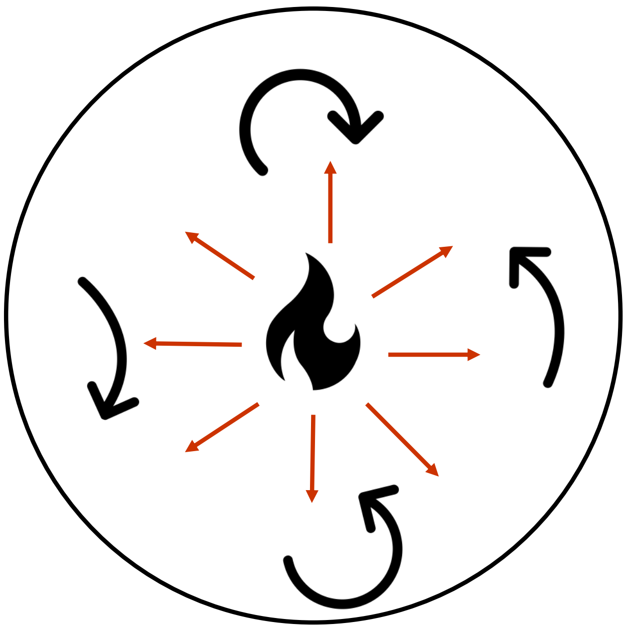
DDT Mechanisms Summary

- Characterized sensitivities of DDT to various parameters
- Introduced novel geometries to isolate contributing factors to DDT
  - Strong reflected pressure wave interactions in unburned fuel
  - Sufficient energy addition resulting in flame acceleration
- Showed that burning surface area is critical to the acceleration required for DDT in a confined, obstructed flow
- Demonstrated that flow separation resulting from sharp edged bodies is what leads to obstructed flows detonating sooner in comparison to unobstructed flows
- Applied more detailed chemical kinetics

UNDERLYING FLOW PARAMETER INFLUENCE ON PROPAGATION

A.M. Coates, S.L. Lawrence, D.L. Mathias, and B.J. Cantwell. Numerical study of hydrogen-oxygen flame speed sensitivities in support of launch vehicle explosion risk modeling. Combustion and Flame, Submitted 2020.

Introduction

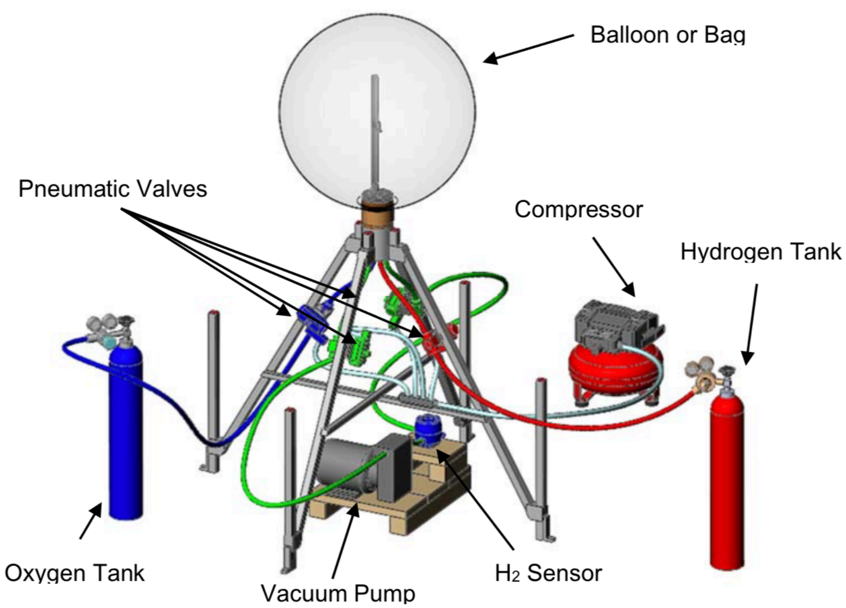


Hydrogen-Oxygen Mixture

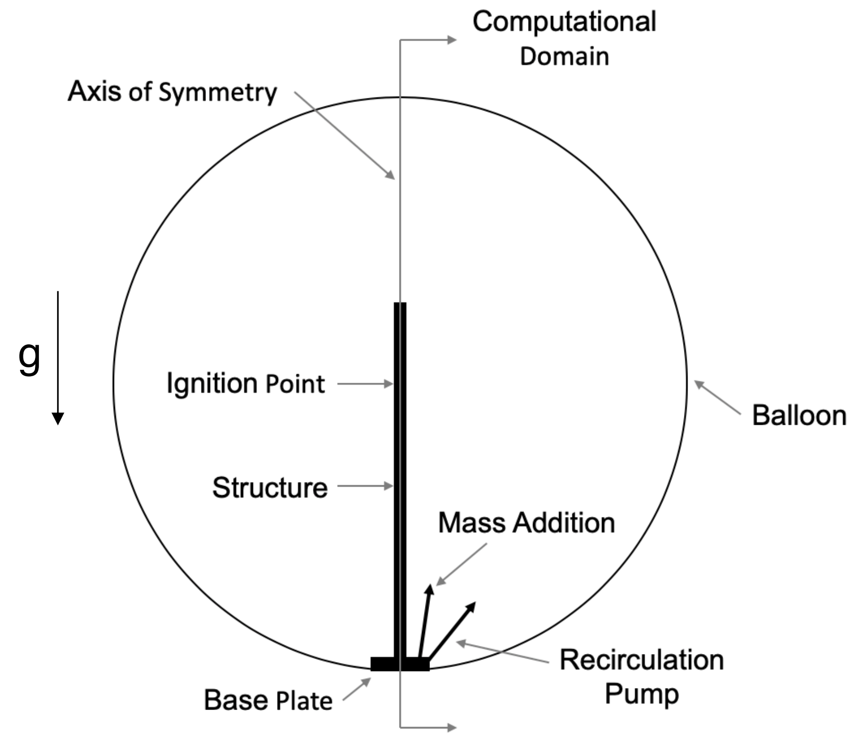
- Initial pressure
- Initial velocity distribution
- Mixture ratio
- Flame acceleration discussion

Geometry

- Geometry representative of Hydrogen Unconfined Combustion Test Apparatus (HUCTA) experiments conducted at MSFC



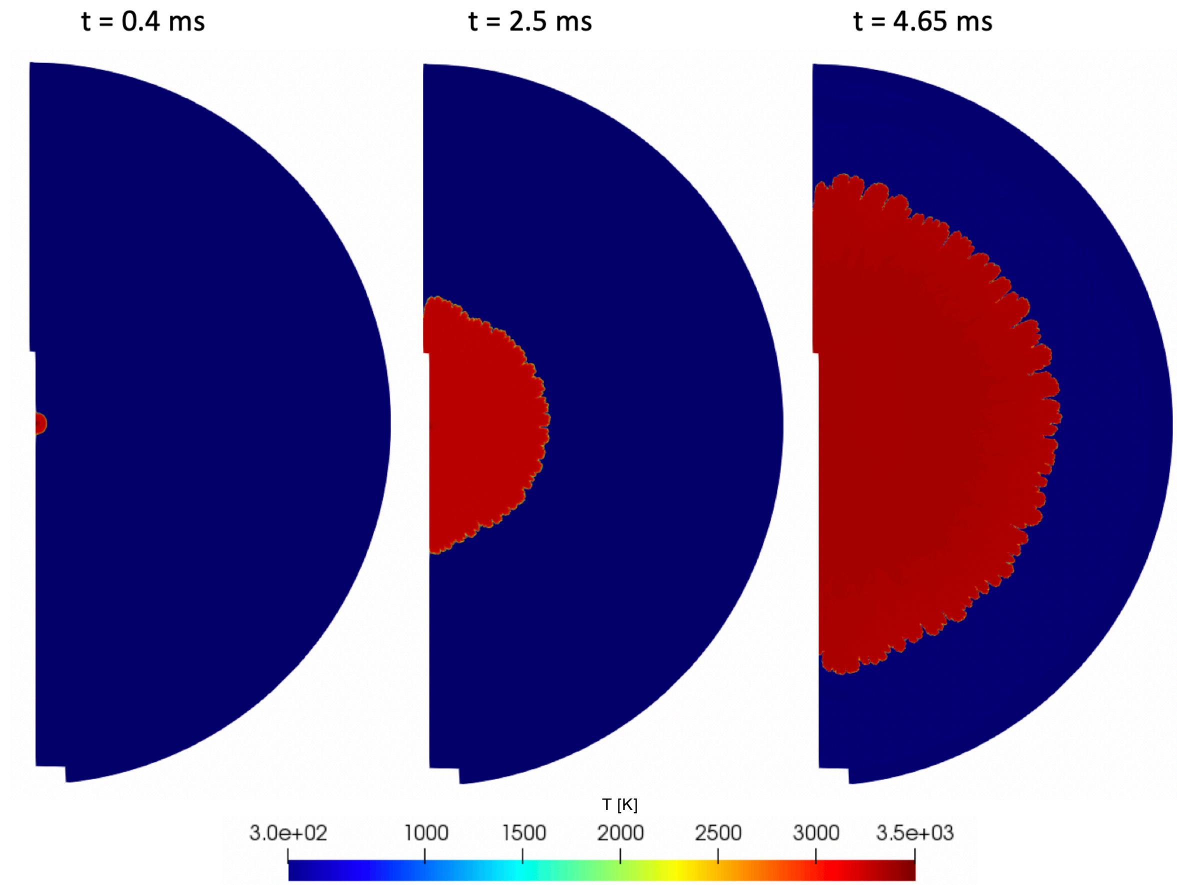
E. Richardson, T. Skinner, J. Blackwood, M. Hays, M. Bangham, and A. Jackson. An experimental study of unconfined hydrogen/oxygen and hydrogen/air explosions. 46th Joint Army-Navy-NASA-Air Force (JANNAF) Combustion Conference, 2014.



Initial Pressure Variation

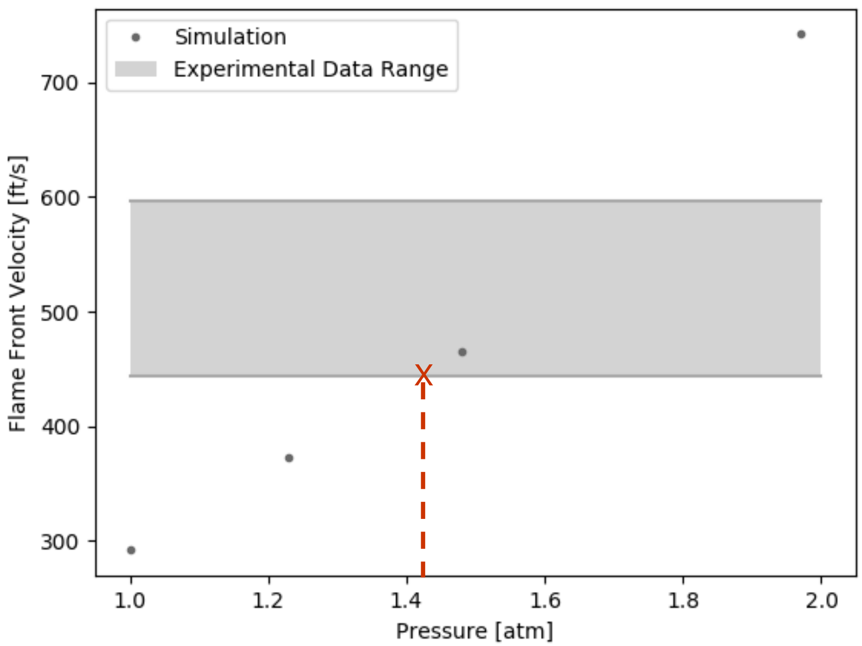
Stoichiometric (ϕ = 1)
P = 125 kPa
Hydrogen-Oxygen

Temperature Contours



Compare to Experiment

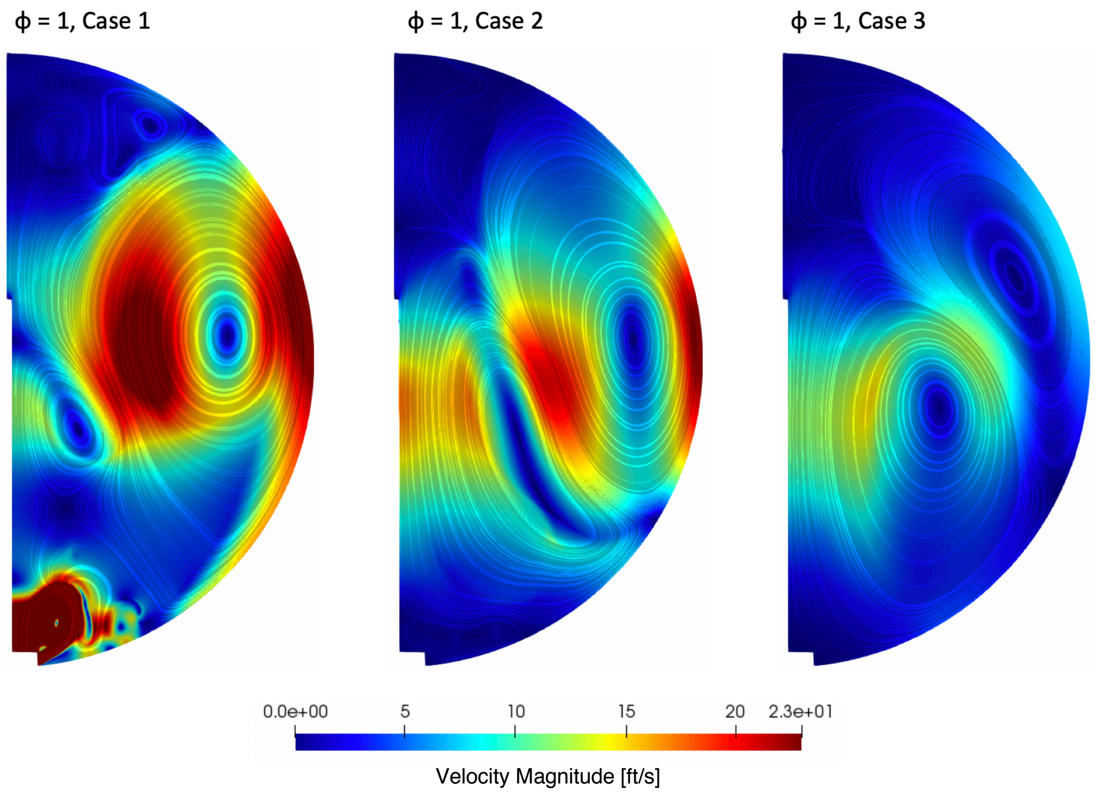
- Quiescent flow, density varies with pressure



NOT PRACTICAL

Initial Velocity and Mixture Ratio Variation

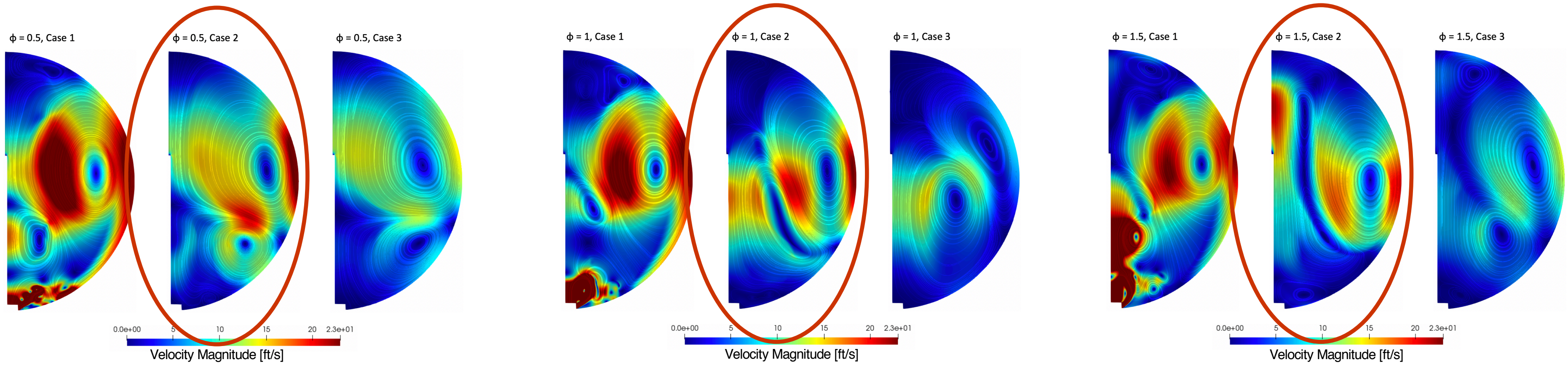
- Simulate adding mass from base plate, introduces velocity into the initial flow



Wait time = 2/3 Fill time

Initial Velocity and Mixture Ratio Variation

- Simulate adding mass from base plate, introduces velocity into the initial flow

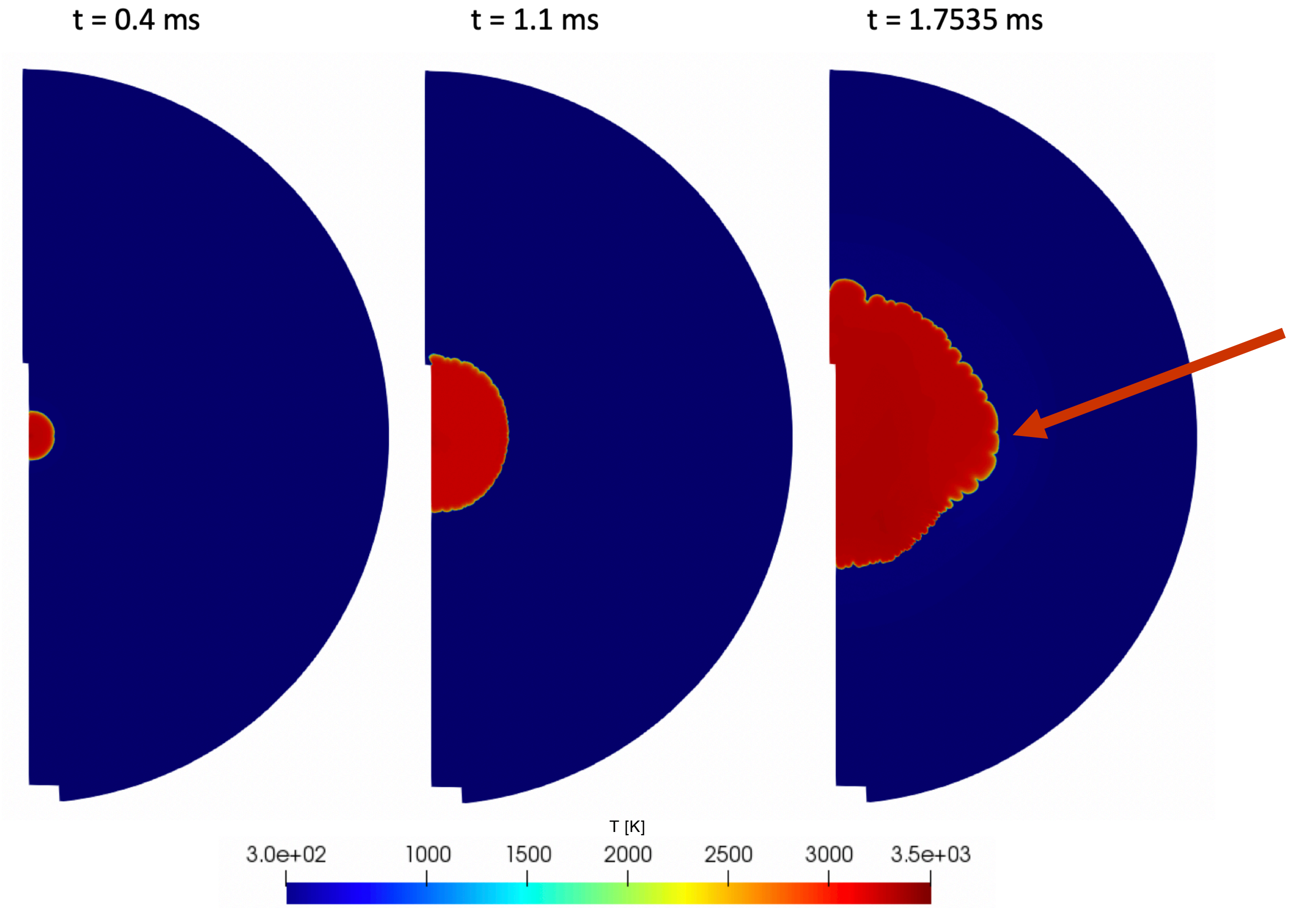


	ϕ = 0.5		**ϕ = 1**		**ϕ = 1.5**	
	Mean [ft/s]	SD	Mean [ft/s]	SD	Mean [ft/s]	SD
Case 1	13.88	6.60	10.67	7.01	12.56	10.18
Case 2	9.83	4.39	10.19	5.09	9.19	4.41
Case 3	8.49	3.95	7.41	3.83	5.12	2.25

Initial Velocity Distribution Variation

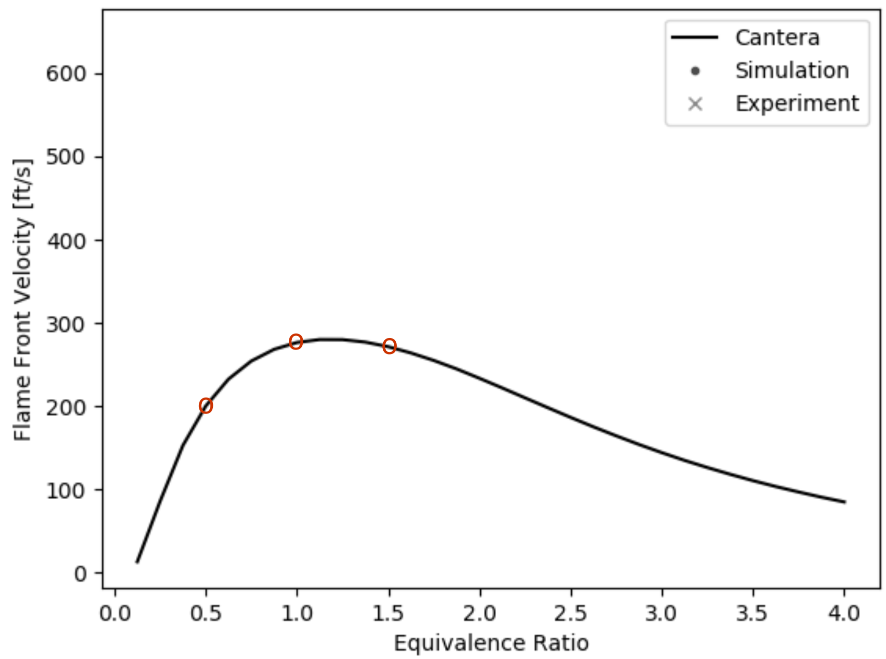
Stoichiometric (ϕ = 1)
Velocity Case 2
Hydrogen-Oxygen

Temperature Contours



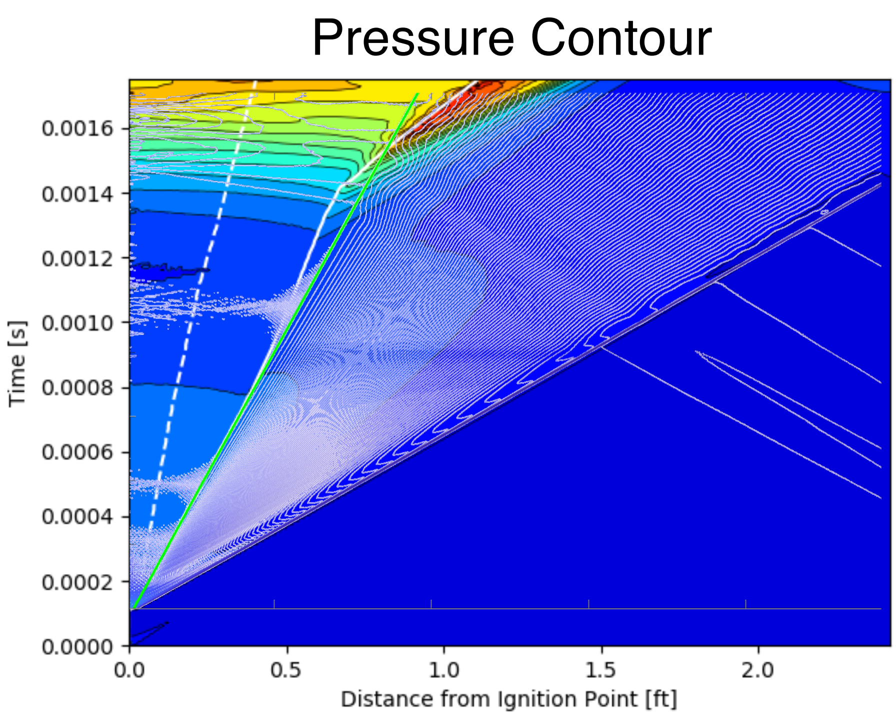
Compare to Experiment

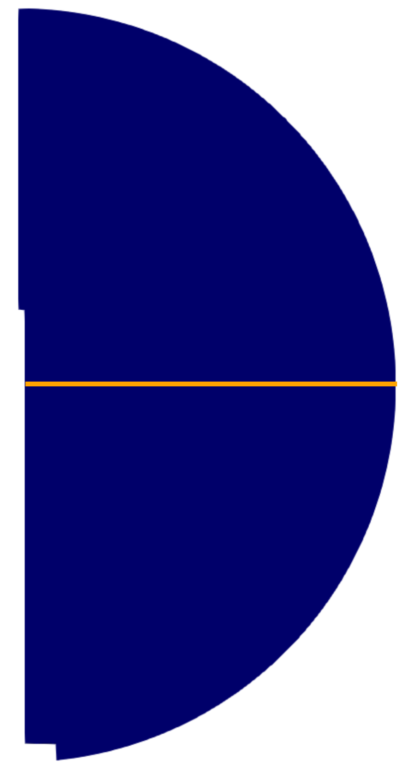
- Stoichiometric mixture with an underlying velocity distribution



Mass addition (velocity) important!

Compare to Model



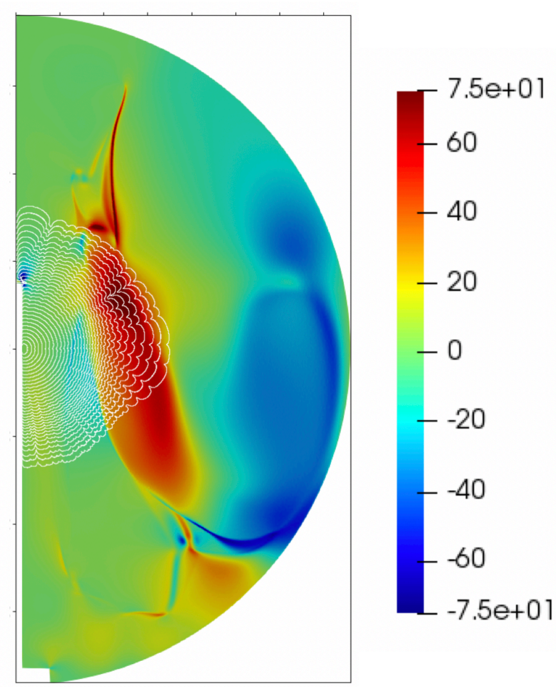


Stoichiometric (ϕ = 1), Case 2

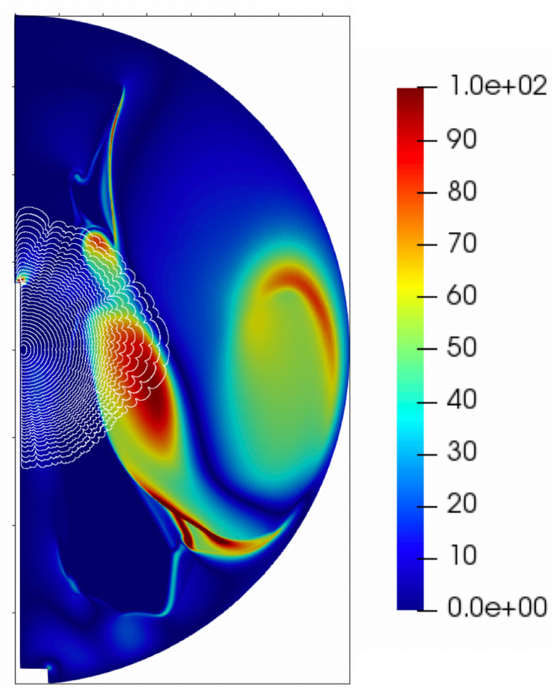
Flame Acceleration Discussion

- Of the variations, **velocity distribution dominated** the flame propagation

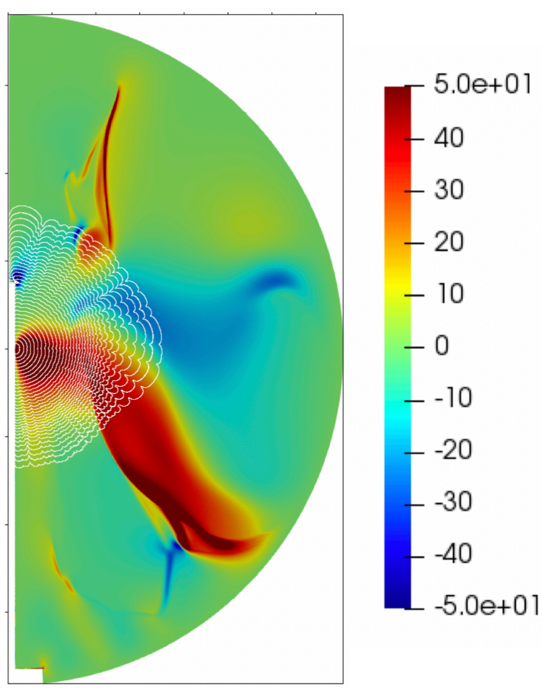
Strain Rate



Vorticity Magnitude



Radial Velocity Gradient



Flame Acceleration Discussion

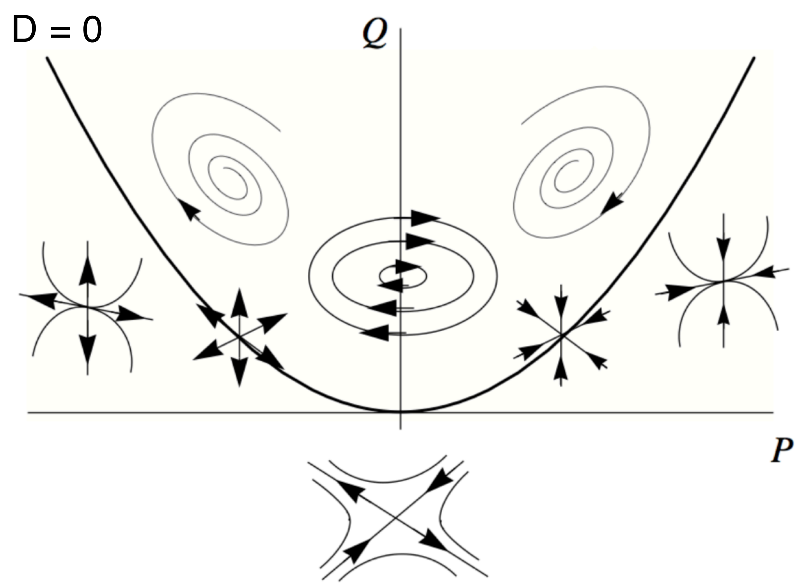
- Classified the flow using 2D elementary flow patterns determined by invariants of the gradient tensor of the velocity field

$$A_{ik} = \frac{\partial U_i}{\partial x_k}$$

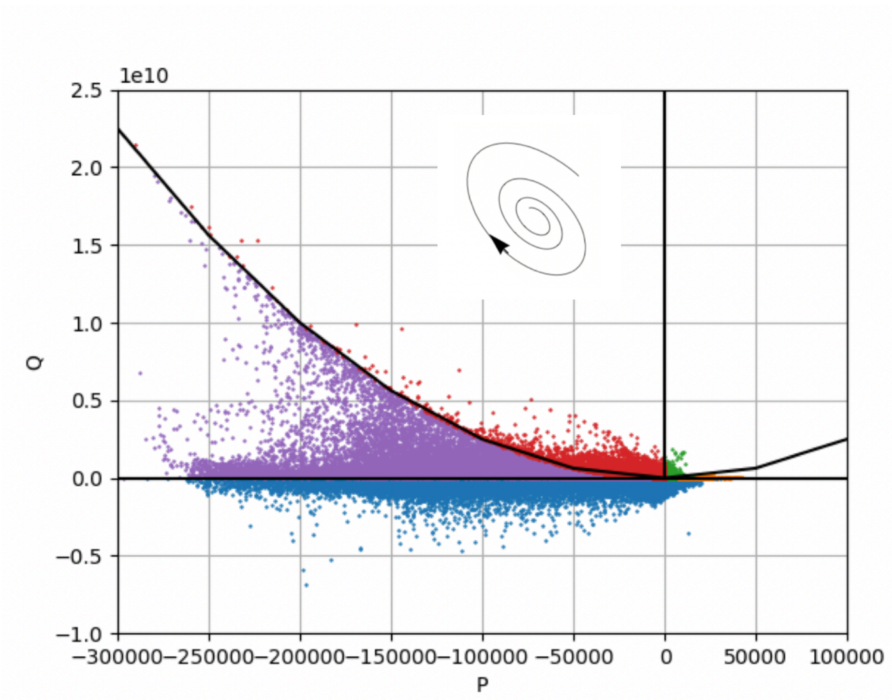
$$P = -A_{ii} = -\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)$$

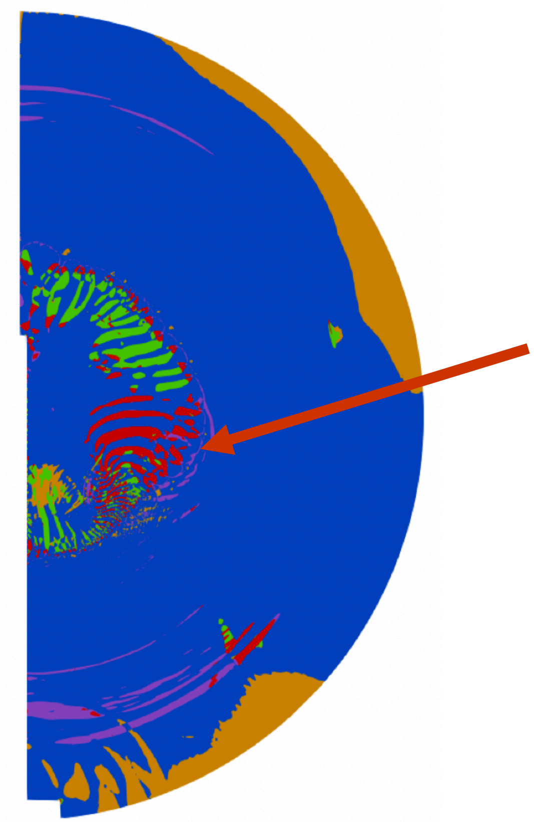
$$Q = Det(A_{ik}) = \frac{\partial u}{\partial x}\frac{\partial v}{\partial y} - \frac{\partial v}{\partial x}\frac{\partial u}{\partial y}$$

$$D = Q - \frac{P^2}{4}$$



Flame Acceleration Discussion





Underlying Flow Summary

- Characterized which underlying parameters the flame speed is most sensitive to
- Demonstrated that interactions with underlying velocity distributions lead to flame acceleration and deformation, significantly affecting the flame speed
- Applied the idea of invariants of the velocity gradient tensor and elementary flow patterns to burning flames
- Confirmed that the current engineering model is good for cases with limited flow features, and identified indicators of acceleration that could be used in non-quiescent flows
- Proposed important variables to be reported when testing or modeling such as initial velocity distribution

SUMMARY

Overall Conclusions

- Obstacle shape
- Number of obstacles
- Ignition source
- Initial conditions

STUDY 1 →

Scenarios with limited sharp edge obstacles and ignition sources at lower densities, pressures, and temperatures reduce the risk of DDT

- Initial Pressure
- Initial velocity distribution
- Mixture ratio

STUDY 2 →

Scenarios with features in the flow lead to local accelerations that increase flame speed and overpressure. Parameters like vorticity and invariants may be effective indicators in modeling

Overall Contributions

- Addressed many of the complex aspects of flame propagation modeling
- Tested a wide variety of parameters and geometries over a range of scenarios relevant to launch vehicle risk assessment modeling
- Characterized flame speed sensitivities
- Introduced novel geometries and analysis methods to isolate contributing factors to flame acceleration
- Applied more detailed chemical kinetics
- Provided insight on when current models are good and when higher fidelity models may be useful, improving future risk assessment modeling

Questions?