Ignition of Hydrogen-Air Mixtures by Moving Heated Particles

J. Melguizo-Gavilanes, S. Coronel, R. Mével and J.E. Shepherd

Explosion Dynamics Laboratory
Graduate Aerospace Laboratories of the California Institute of Technology (GALCIT)
Pasadena, CA US

6th International Conference on Hydrogen Safety - Yokohama, Japan
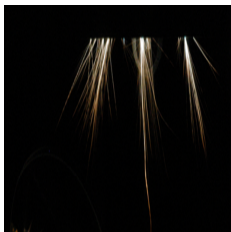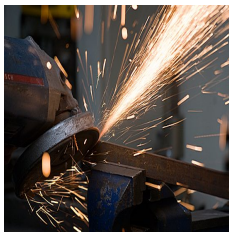
October 2015

Caltech

NSERC
CRSNG

Outline

Motivation - Why is it important ?

Motivation
Improved understanding of ignition hazards

Aircraft fuel tank safety [1]

Manufacturing safety [2]

Mining safety [3]

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1. Simulated lightning strike on composite coupon performed at Boeing
2. Mechanical sparks from cutting and reshaping processes
3. Hot particles of decomposed explosive and casing

Outline

Experimental work

Classical Experimental Work
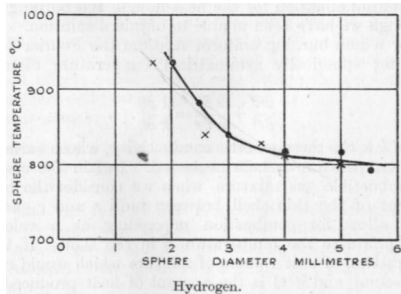In the 1930's motivated by coal-mining operations - frictional sparks (moving heated particles)

Figure 5 : effect of particle diameter [1]

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1. R.S. Silver. *Phil. Mag. J. Sci.*, 23(156) : 632-657/1937.

Experimental work

More Recent Experimental Work
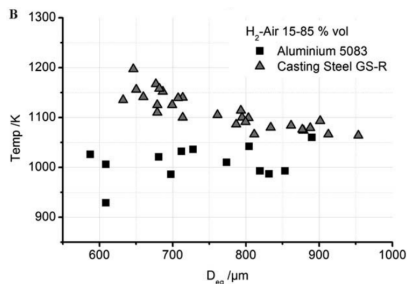Ignition of gaseous mixtures by submillimeter size stationary hot particles
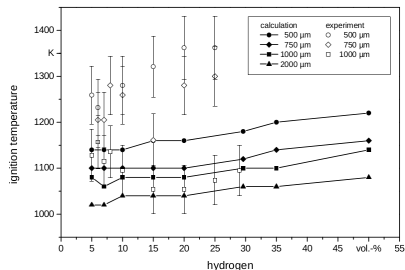

Figure 2b : effect of particle material [2]

Figure 4 : effect of mixture concentration [3]

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2. D. Roth et al. *Combust. Sci. Techno.*, 186 :10-11/2014.
3. M. Beyer and D. Markus. *8th ISHPMIE Yokohama, Japan*, 2010.

Experimental work

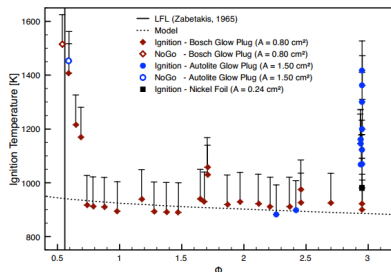## Previous & Current Experimental Efforts at Caltech
Ignition of *n*-hexane mixtures
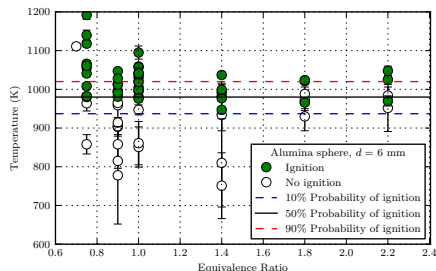

Figure 3.15 : transiently heated surfaces [4]

Figure : moving heated spheres [5]

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4. P.A. Boettcher. *Ph.D Thesis. Caltech*, 2012.
5. S. Coronel. *Ph.D Thesis. Caltech (in preparation)*, 2015.

Numerical work

Some Previous & Current Numerical Efforts
1D Simulation assuming spherical symmetry, quiescent atmosphere and no-thermally induced convection
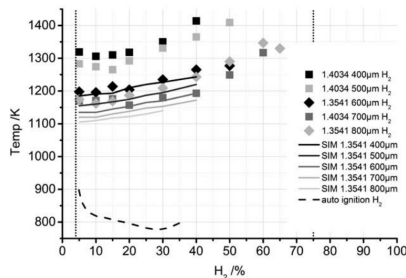

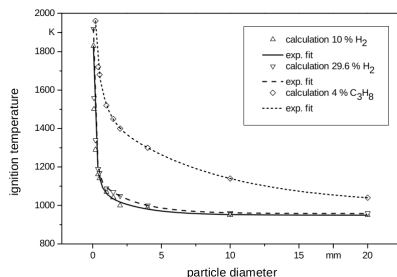**Figure 3b : Effect of mixture concentration** [6]

Figure 8 : Effect of particle size [7]

6. D. Roth et al. *Combust. Sci. Techno.*, 186 :10-11/2014.
7. M. Beyer and D. Markus. *8th ISHPMIE Yokohama, Japan*, 2010.

Theoretical Work

Analysis

- C.K. Law [8] - Stagnation-point ignition of a premixed combustible and ignition of a combustible by hot particles (B.L. equations, one-step irreversible reaction and high activation energy limit)
- Y. B. Zel'dovich [9] - Ignition of a fuel mixture flowing around an object (B.L. equations, one-step irreversible reaction, Dorodnitsyn transformation, no assumptions made w.r.t. activation energies, complete analytical investigation of the system was impossible)
- More recently Golovin, A.M. and Golovin, A.M & Rudakova, N.B. [10] with similar simplifying assumptions ...

8. *Int. J. Heat Mass Transfer.*, 21 : 1363-1368/1978a. ; *AIAA Journal*, 16(6) :628-630/1978b.
9. *The Mathematical Theory of Combustion and Explosions*, 1985.
10. *High Temperature*, 1996/1998.

Outline

Goal

Objective

- Explain the dynamics of ignition of combustible gases by inert moving heated spheres when close and far from the ignition limit
- Study the competition between diffusive and convective losses, and chemical heat release to unravel the complex physics and chemistry at play within the boundary layer during the ignition process
- Explore the quantitative prediction of ignition thresholds

Outline

Physical Model - Governing Equations

Reactive Navier-Stokes with temperature dependent properties
(μ : Sutherland Law, $\alpha = k/c_p$: Eucken Relation, c_p : JANAF)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g}$$

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (\kappa/c_p \nabla h) + q_{chem}, \ \ (Le = 1)$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \Omega_i$$

with $p = \rho \bar{R} T, \ \ \tau = (p + \frac{2}{3}\mu \nabla \cdot \mathbf{u})\mathbf{I} + \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$

$$h = \sum h_i Y_i, \ \ q_{chem} = \sum h_i \Omega_i, \ \ \Omega_i = \rho d Y_i/dt$$

Challenges

- Wide range of temporal and spatial scales involved
    - Size of experimental aparatus ($\mathcal{O}(m)$)
    - Hydrodynamic length scales - Boundary layer thickness ($\mathcal{O}(\mu m) - \mathcal{O}(mm)$)
    - Chemical induction/ignition times ($\mathcal{O}(s)/\mathcal{O}(ms)$) and flame thickness ($\mathcal{O}(\mu m)$)
- Size of detailed chemical kinetic mechanisms
    - Hydrocarbon fuels conventionally used for transportation comprise thousands of reactions and hundreds of species (e.g. *n*-hexane detailed mechanism : 2581 reactions and 457 species)

Physical Model - Hydrogen Chemistry

Mével's Mechanism (9 species and 21 reactions) [11]
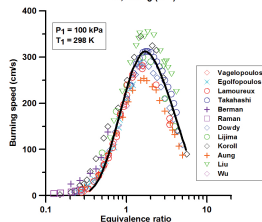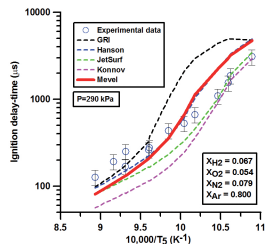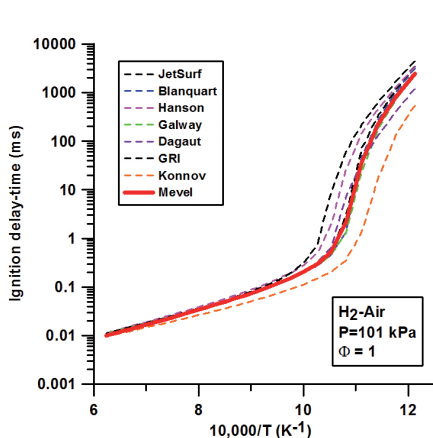
11. R. Mével et al. *P. Combust. Inst.*, 32 & 33 / 2009 & 2011

Approach

- 2D simulation of reactive viscous flow using the Open source Field Operation And Manipulation (OpenFOAM) toolbox [12]
- Spatial discretization done with Finite Volumes (FV)
- Pressure-velocity coupling achieved using PIMPLE (PISO + SIMPLE) [13]
- Implementation of time dependent boundary conditions to reproduce actual experimental conditions
- High Performance Computing - resources provided by the Extreme Science and Engineering Discovery Environment (XSEDE) supported by the National Science Foundation (NSF)

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12. H.G. Weller et al. *J. Comput. Phys.*, 12 : 620-631/1998.
13. I. Demirdzic and Péric. *Int. J. Numer. Meth. Fl.*, 16 : 1029-1050/1993.

Experimental setup, initial & boundary conditions
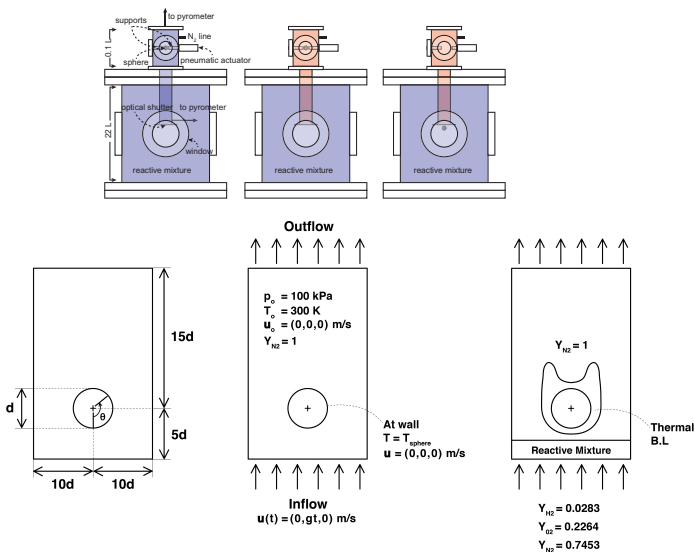
Nature of flow before contact with reactive mixture
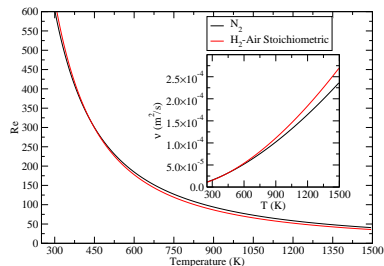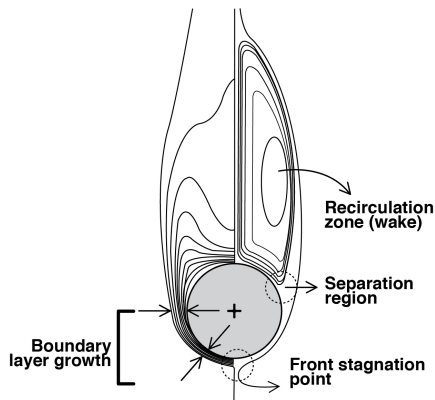
Comparison with non-reactive experiments
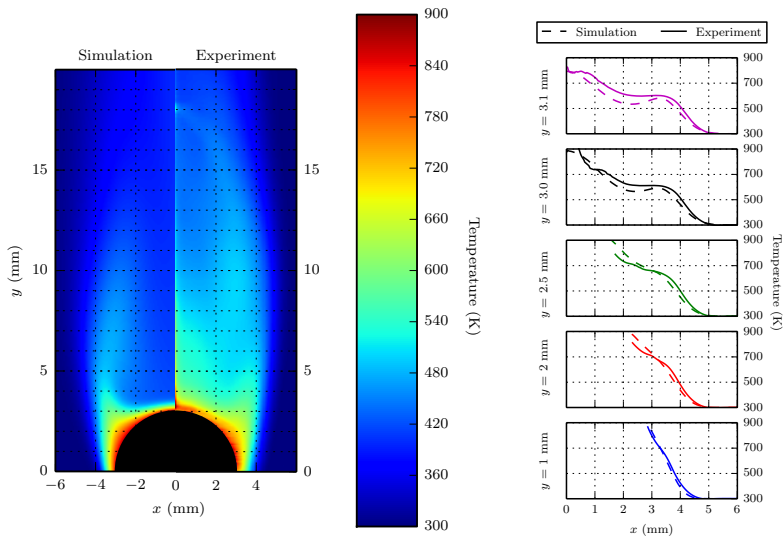
Outline

Flow structure - boundary layer development
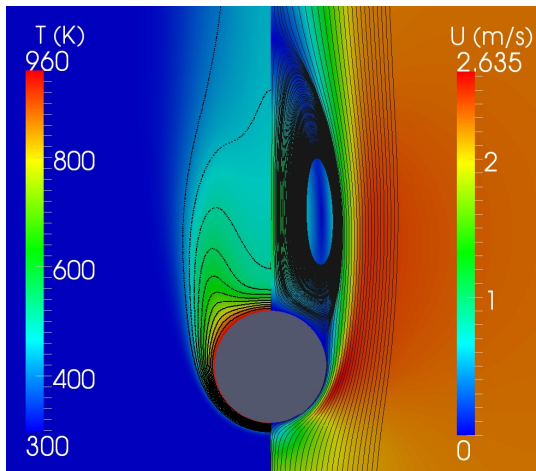
**Temperature and velocity fields, temperature isocontours
and streamlines before contact with reactive mixture**

When does ignition take place ?
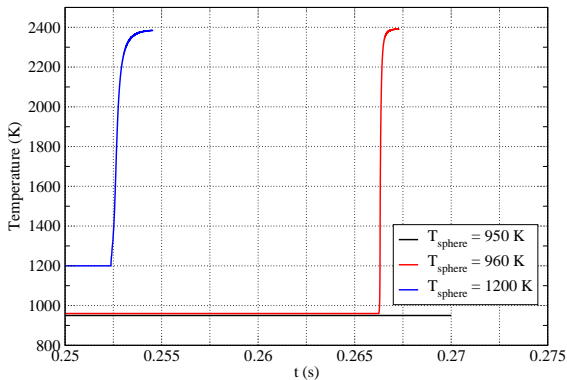
Temperature maximum in computational domain
$\tau_{\mathbf{ign}} = \mathbf{T_{sphere}} + \mathbf{150K}$

When does ignition take place ?
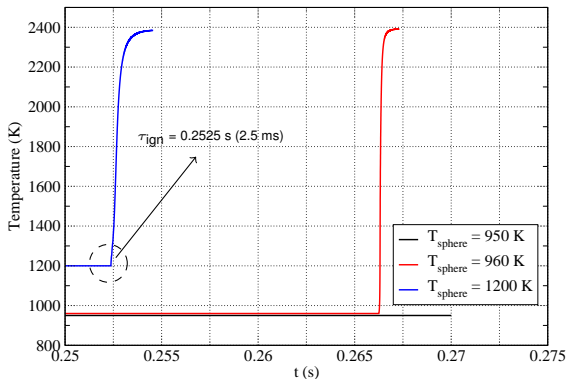
Temperature maximum in computational domain
$\tau_{ign} = T_{sphere} + 150K$

When does ignition take place ?
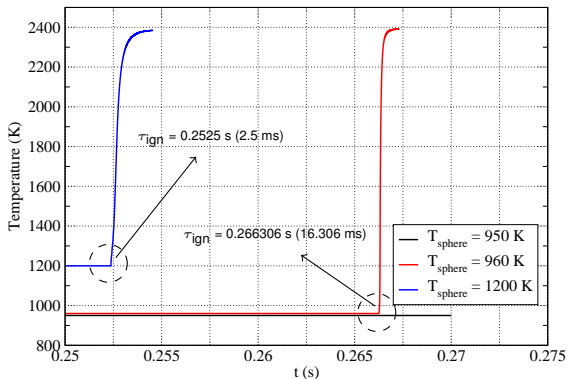
Temperature maximum in computational domain
$\tau_{ign} = T_{sphere} + 150K$

Where does ignition take place ? (1/8)

T_{sphere} = 1200 K - Ignition Evolution
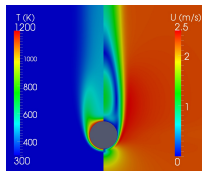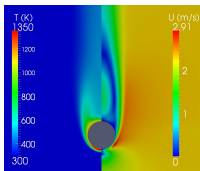
$t = 0.25237\,s$ $t = 0.25250\,s$ $t = 0.25275\,s$ $t = 0.2530\,s$
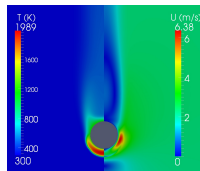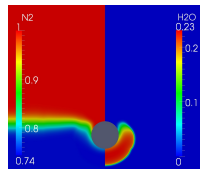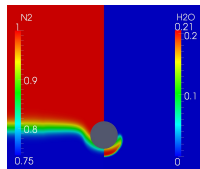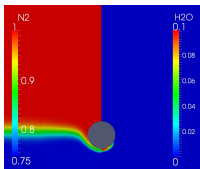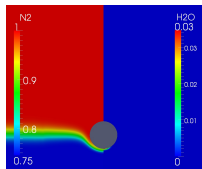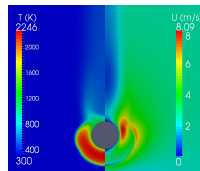

Shortly before ignition   Ignition   Flame kernel formation   Flame propagation

Where does ignition take place ? (2/8)

T_sphere = 1200 K
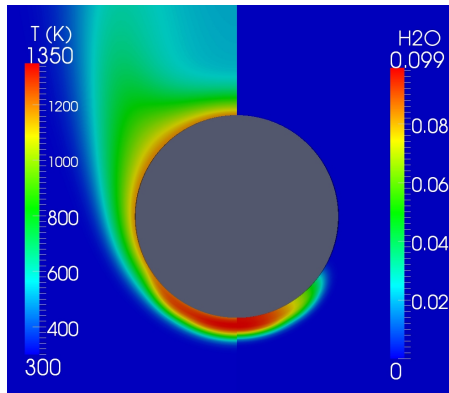
Closeup to ignition location - $\theta = 0°$

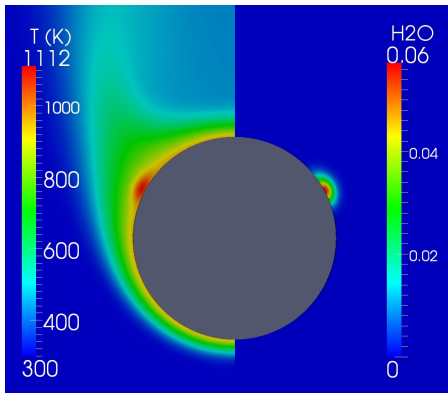# Where does ignition take place ? (3/8)

T_{sphere} = 1000 K - Ignition Evolution
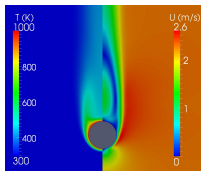
$t = 0.254354\,s$ $t = 0.254386\,s$ $t = 0.254466\,s$ $t = 0.25475\,s$
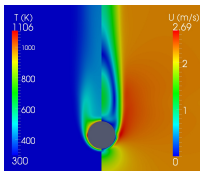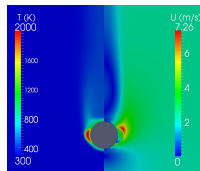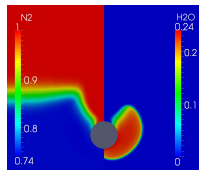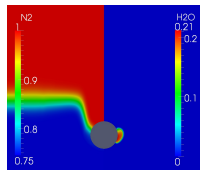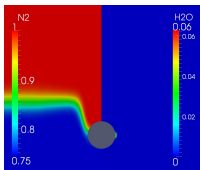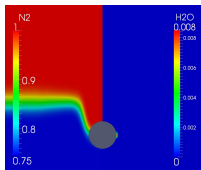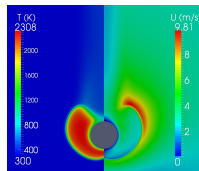
Shortly before ignition   Ignition   Flame kernel formation   Flame propagation

Where does ignition take place ? (4/8)

T$_{sphere}$ = 1000 K
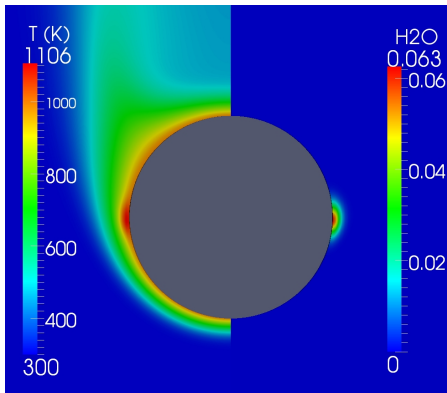
Closeup to ignition location - $\theta = 90°$

Where does ignition take place ? (5/8)

T_{sphere} = 960 K - Ignition Evolution

$t = 0.26625\ s$

$t = 0.266306\ s$

$t = 0.266362\ s$

$t = 0.2665\ s$

Shortly before ignition

Ignition

Flame kernel formation

Flame propagation
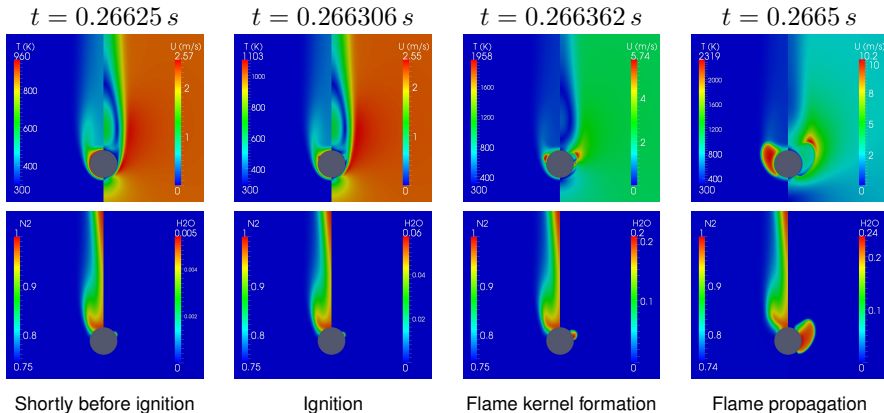
Where does ignition take place ? (6/8)

T$_{sphere}$ = 960 K

Closeup to ignition location - $\theta = 115°$ (threshold)

Where does ignition take place ? (7/8)

T$_{sphere}$ = 950 K - No Ignition
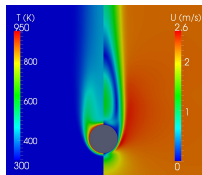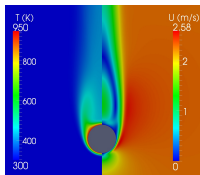
$t = 0.255\,s$ $t = 0.260\,s$ $t = 0.265\,s$ $t = 0.270\,s$
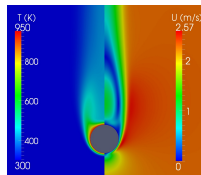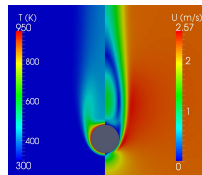
Where does ignition take place ? (8/8)

T$_{sphere}$ = 950 K
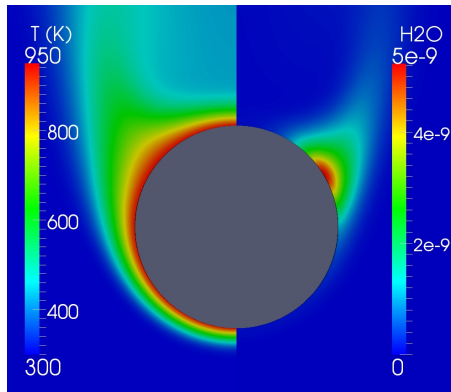
No Ignition

Results Summary
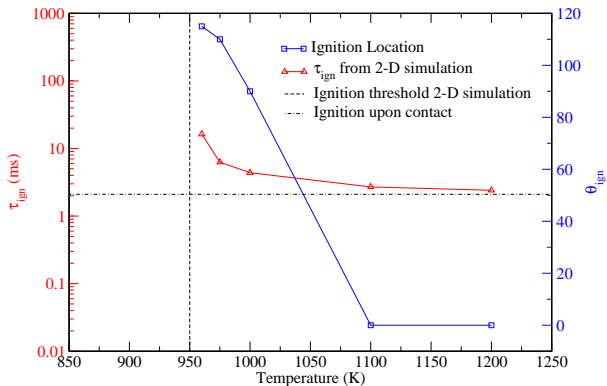
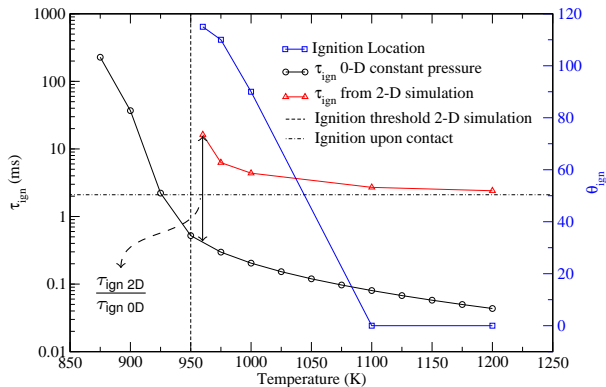**Ignition times and locations from 2D simulations**

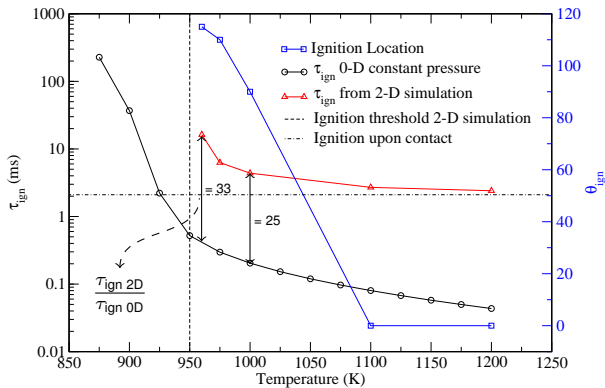# Outline
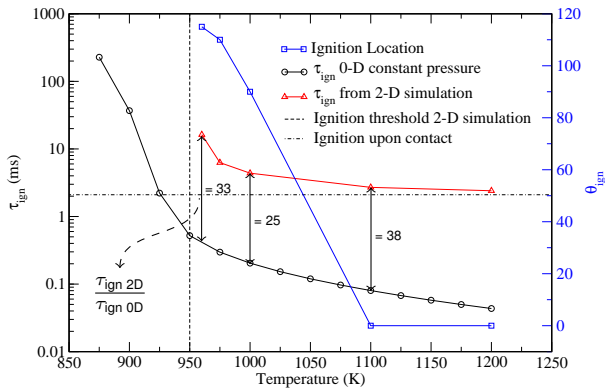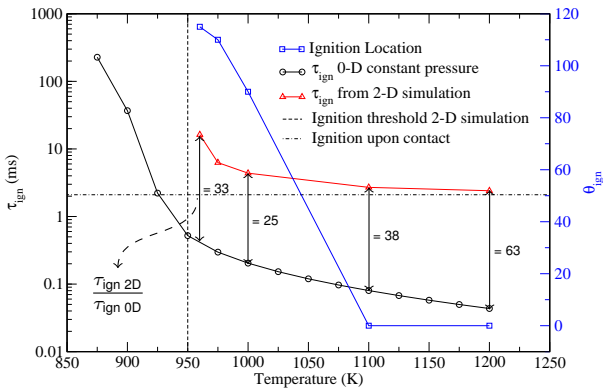
Ignition times analysis

Comparison of 2D and constant pressure ignition times

Ignition times analysis

Comparison of 2D and constant pressure ignition times

Ignition times analysis
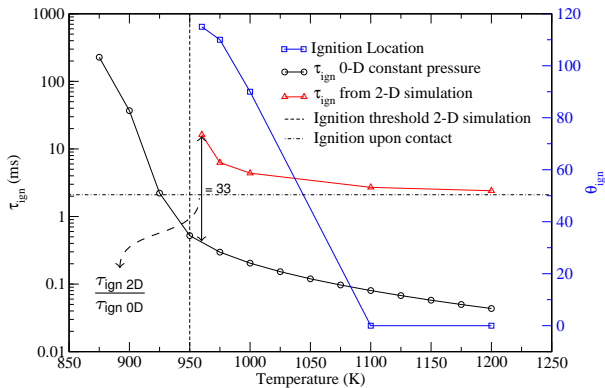
Comparison of 2D and constant pressure ignition times

Ignition times analysis

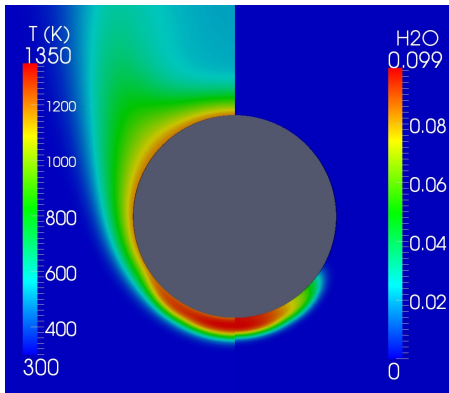**Comparison of 2D and constant pressure ignition times**

Ignition times analysis

Comparison of 2D and constant pressure ignition times

Ignition times analysis

Comparison of 2D and constant pressure ignition times

Energy equation analysis (1/5)

Recall the energy equation

$$\underbrace{\frac{\partial(\rho h)}{\partial t}}_{\text{Sum (---)}} = \underbrace{-\nabla \cdot (\rho \mathbf{u} h)}_{\text{hConvection (—)}} + \underbrace{\nabla \cdot (\kappa/c_p \nabla h)}_{\text{hDiffusion (—)}} + \underbrace{q_{chem}}_{\text{hSource (—)}}$$
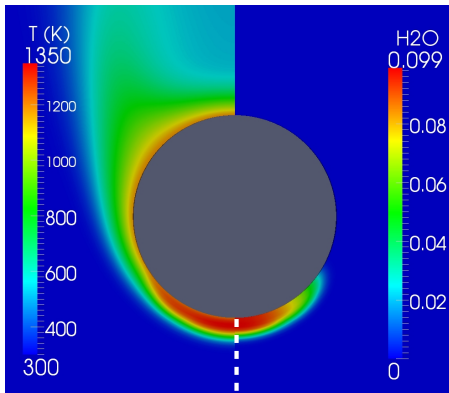
Energy equation analysis (2/5)

T$_{sphere}$ = 1200 K

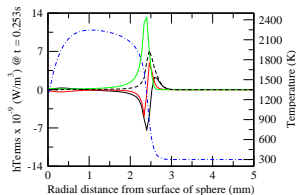**Closeup to ignition location -** $\theta = 0°$

Energy equation analysis (2/5)

T$_{sphere}$ = 1200 K

Closeup to ignition location - $\theta = 0°$
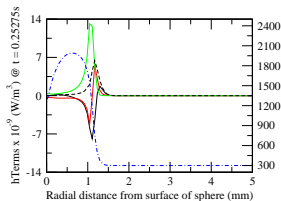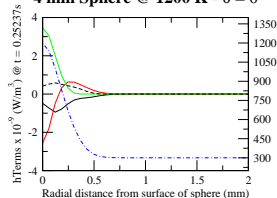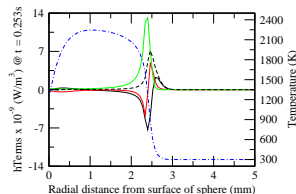
Energy equation analysis (3/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface
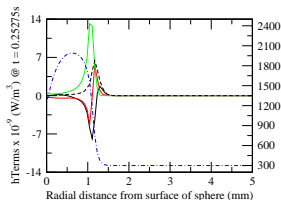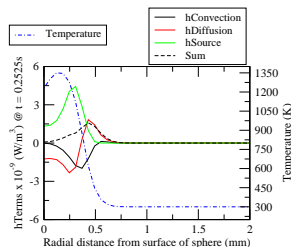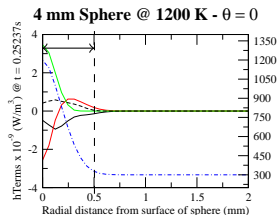
Energy equation analysis (3/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (3/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (3/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (3/5)
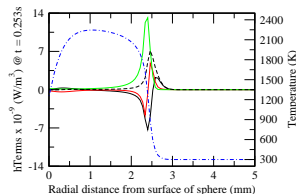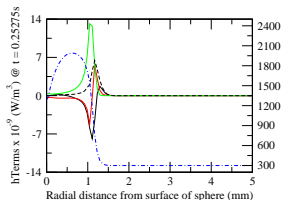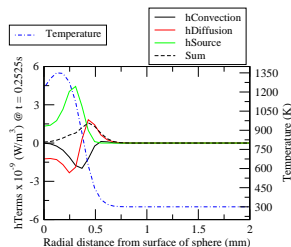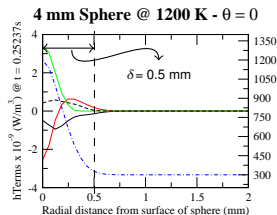

4 mm Sphere @ 1200 K - θ = 0

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (3/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface
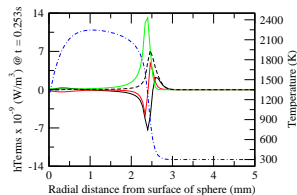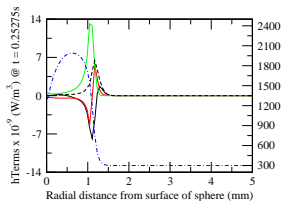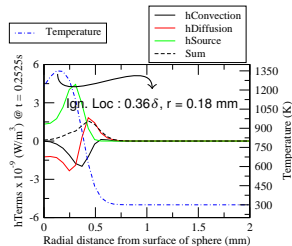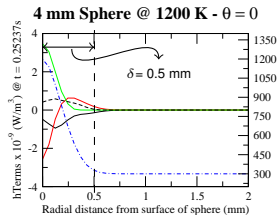
Energy equation analysis (3/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (4/5)

T_{sphere} = 960 K

Closeup to ignition location - $\theta = 115°$ (threshold)

Energy equation analysis (4/5)

T$_{sphere}$ = 960 K

Closeup to ignition location - $\theta = 115°$ **(threshold)**
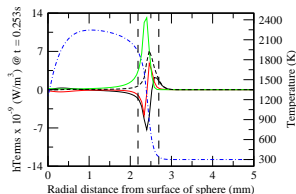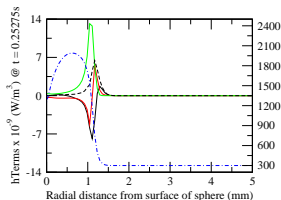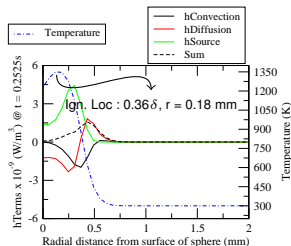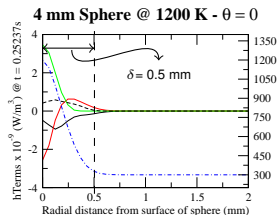
Energy equation analysis (5/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (5/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface
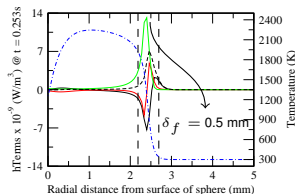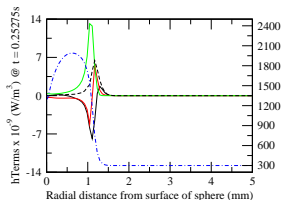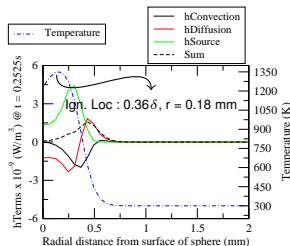
Energy equation analysis (5/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

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Contributions of each term in energy equation and temperature along radial distance from sphere's surface
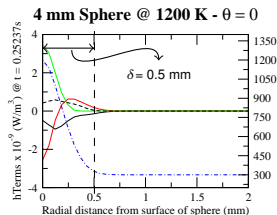
Energy equation analysis (5/5)

Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Energy equation analysis (5/5)

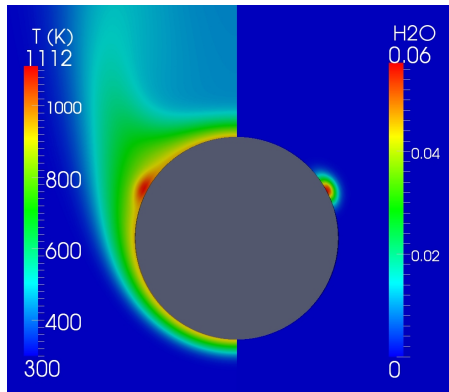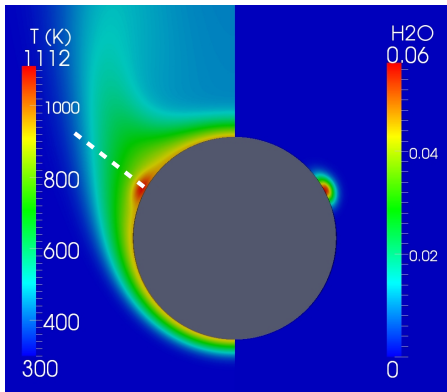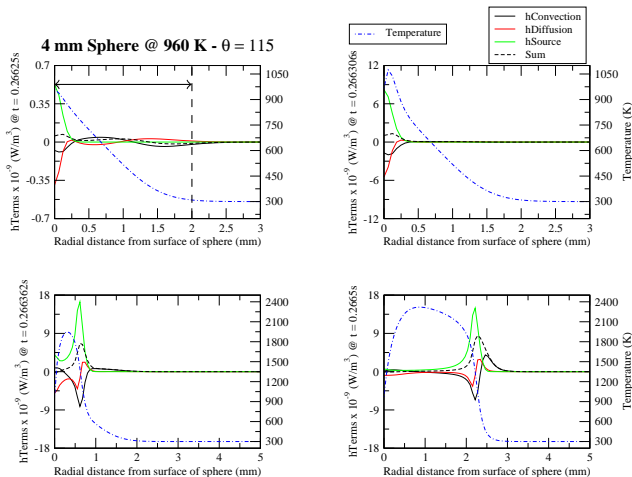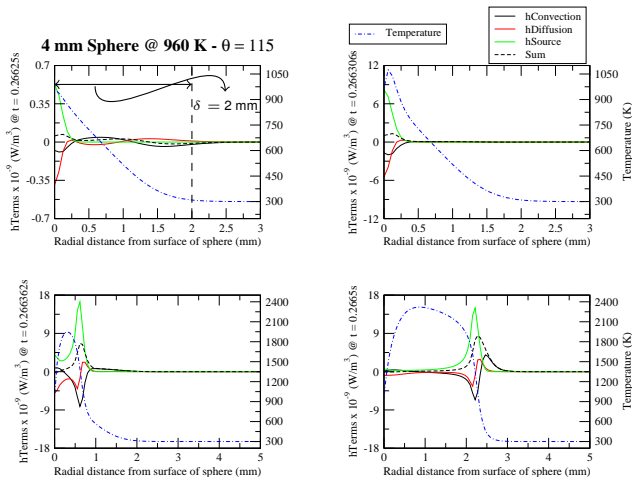Contributions of each term in energy equation and temperature along radial distance from sphere's surface

Temporal evolution near ignition location (1/2)

T$_{sphere}$ = 1200 K
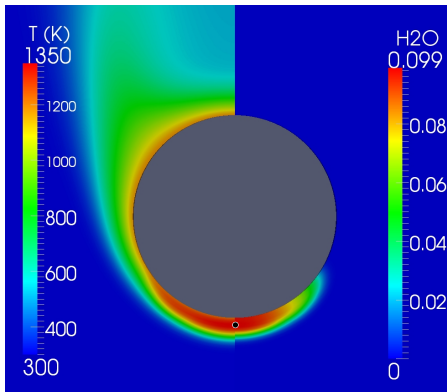
Closeup to ignition location - $\theta = 0°$

Temporal evolution near ignition location (2/2)
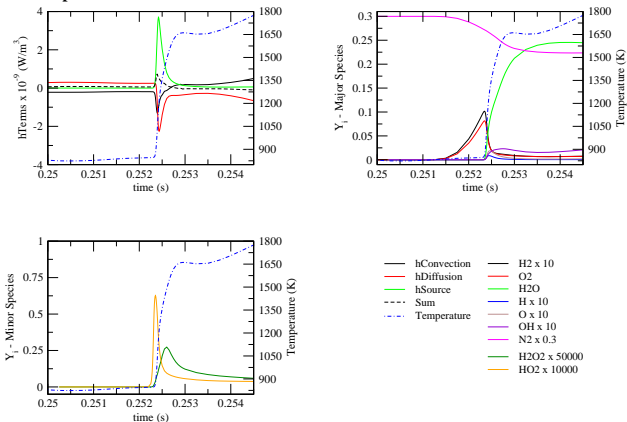
4 mm Sphere @ 1200 K - θ = 0 @ 0.36δ

Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location

Temporal evolution near ignition location (2/2)

4 mm Sphere @ 1200 K - θ = 0 @ 0.36δ
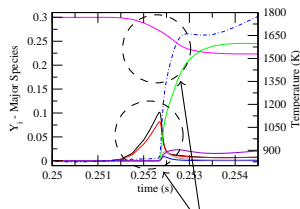
B.L. Flushing - Ignition occurs in more diluted mixture

Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location

Temporal evolution near ignition location (3/4)

T_sphere = 960 K
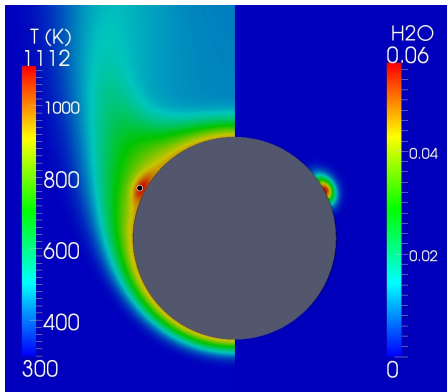
Closeup to ignition location - $\theta = 115°$ (threshold)

Temporal evolution near ignition location (4/4)

4 mm Sphere @ 960 K - θ = 115 @ 0.04δ

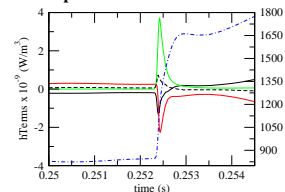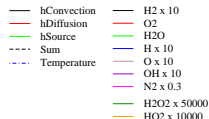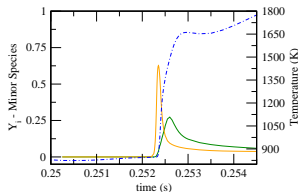**Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location**

Temporal evolution near ignition location (4/4)

Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location
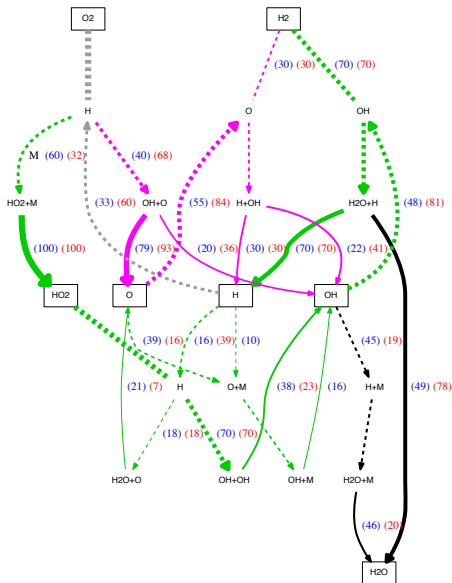
Chemical Pathways

Chemical Pathways

T_{sphere} = 1200K
T_{sphere} = 960K

Box : Species Reservoirs
——— : Reservoir Inputs
--- : Reservoir Outputs

——— : Chain-branching
——— : Mixed pathways
——— : Non-chainbranching

At high T :
OH radicals mostly produced by chain-branching processes (77%)
R_1 : O_2 + H = OH + O
R_2 : H_2 + O = H + OH
Non-chain branching through Path 1 (23%)

Chemical Pathways

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R_2 : H_2 + O = H + OH
Non-chain branching through Path 1 (23%)

At low T :
Chain-branching processes significantly less (42%)
Non-chain branching processes
Path 1 (38%) :
R_5 : H + O_2(+M) = HO_2(+M)
R_3 : HO_2 + H = OH + OH
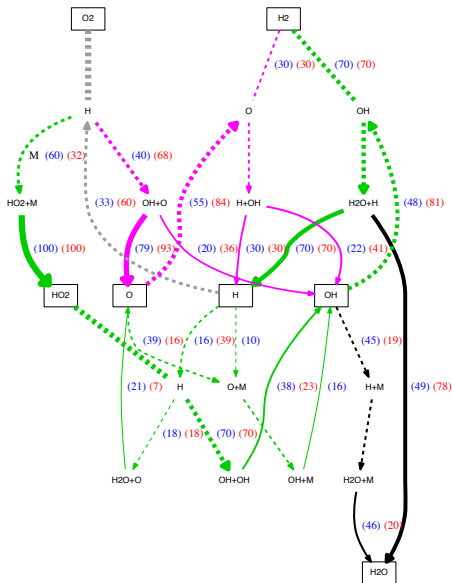**Path 2 (16%) :**
R_6 : H + O(+M) = OH(+M)

Outline

Closing Remarks (1/2)

- Quantitative prediction of ignition thresholds for hot surfaces require a detailed model that includes correct initial and boundary conditions to capture important features such as boundary layer separation, and energy transport processes

- Ignition occurs within the thermal boundary layer at a location that depends strongly on temperature

- Large differences observed between 2D and 0D ignition times suggests that simplified models based on comparison of residence times with ignition delay times are inappropriate

- As the temperature decreases to the ignition threshold, non-chain branching chemical pathways are favored over chain branching processes

Closing Remarks (2/2)

- Two distinct behaviors observed :
  - Far from the ignition threshold
    - Reaction starts shortly after contact with reactive mixture
    - Ignition occurs between the front stagnation point and separation region depending upon the sphere's surface temperature
    - Ignition time is very short and takes place in a more diluted mixture compared cases close to the ignition threshold
  - Closer to the threshold
    - Rate of heat deposition into the gas not high enough to trigger fuel conversion during transit from the front stagnation point to the separation region
    - Boundary layer separation results in a zone of slower moving gas, where reactive mixture is "confined", conduction of heat takes place readily and convective losses are minimal

Conclusion

Not only does flow separation play an important role in hot particle ignition, but also when considering different geometries