

# Hot surface ignition of hydrogen-air mixtures

**J. Melguizo-Gavilanes, R. Mével and J.E. Shepherd**

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

6<sup>th</sup> International Conference on Hydrogen Safety - Yokohama, Japan

October 2015

**Caltech**



# Outline

- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

# Motivation - Why is it important ?

## Motivation

Improved understanding of ignition hazards (e.g. hot surface ignition)



Aircraft safety



Nuclear safety



Chemical proc. safety



Mining safety

# Outline

1 Motivation

2 Previous Work

3 Current Experimental Work

4 Goal

5 Physical Model, Numerical Approach and Simulation Parameters

6 Results

7 Discussion

8 Closing Remarks

# Experimental work

## Classical Experimental Work<sup>1</sup>

In the late 1920's motivated by coal-mining operations using heated bars

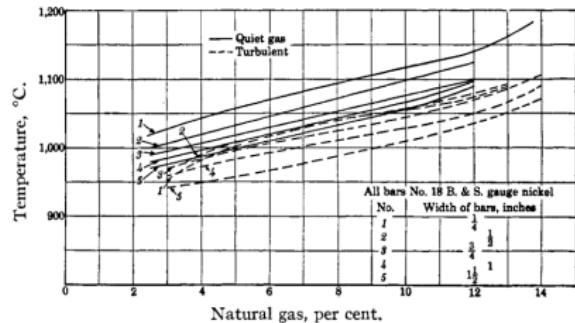


Figure 1 : effect of bar size (nickel)

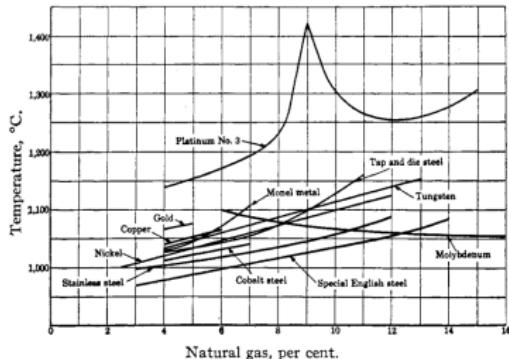


Figure 2 : effect of bar material

1. Coward and Guest. *J. Am. Chem. Soc.*, 49(10) : 2479-2486/1927.

# Experimental work

## More Recent Experimental Work

Kutcha et al. (1965), Kutcha (1985), Smyth & Bryner (1997), Boettcher (2012)

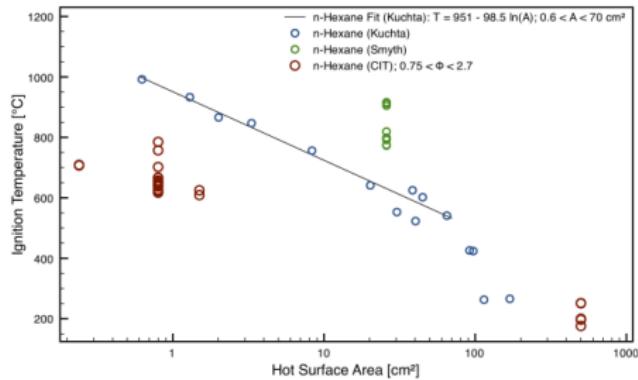


Figure 3.26 : effect of hot surface size<sup>2</sup>

# Experimental work

## Previous Experimental Efforts at Caltech<sup>3</sup>

Ignition of *n*-hexane mixtures using a commercial glowplug

$$p = 101 \text{ kPa}, \Phi = 1.74$$

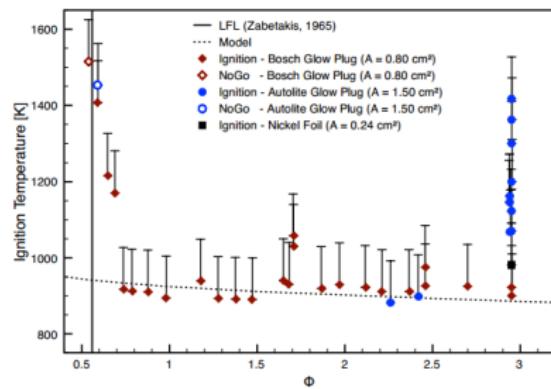


Figure 3.15 : effect of mixture composition

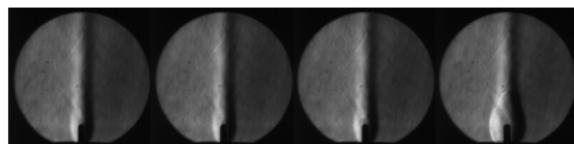


Figure 3.40 : schlieren visualization (edited)

# Theoretical Work

## Analysis

Typical approach is to reduce the problem to a 1D steady energy equation with heat release from chemical reactions

- N.N. Semenov<sup>4</sup> - derived analytical expression for ignition temperature as function of surface area
- Kutch et. al<sup>5</sup> - extended and simplified Semenov's findings
- B.F. Gray<sup>6</sup> - used Semenov's theory to investigate effect of S/V on ignition of NTC fuels
- C.K. Law and H.K. Law<sup>7</sup> - solved the steady boundary layer equations for mixtures with high activation energies using matched asymptotics
- N.M. Laurendeau<sup>8</sup> - proposed simple model to estimate minimum ignition temperature

---

4. *Thermal Theory of Combustion and Explosion*, 23 : 1940.

5. *J. Chem. Eng. Data*, 10(3) : 282-288/1965.

6. *Combust. Flame*, 14(1) : 113-115/1970.

7. *J. Fluid Mech.*, 92(01) : 97-108/1979.

8. *Combust. Flame*, 46 : 29-49/1982.

# Numerical work

## Some Previous Numerical Efforts

- R.K. Kumar<sup>9</sup> - 1D unsteady model to study hot surface ignition of hydrogen-oxygen-diluent mixtures
- J. Adler<sup>10</sup> - 2D steady simulations of ignition by a circular hot spot
- P.B. Boettcher<sup>11</sup> - 2D transient simulations to capture LFL with tabulated chemistry and study the effect of surface area on ignition temperature

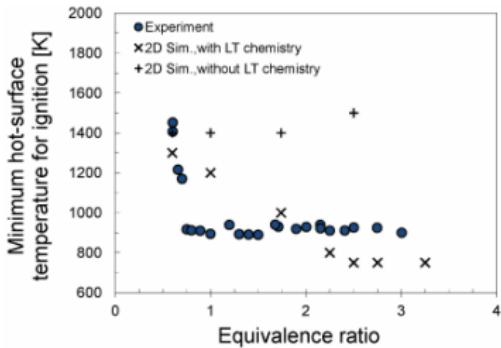


Figure 3.23 : hot surface ignition temperature from tabulated chemistry simulations<sup>11</sup>

- 
9. *Combust. Flame*, 75(2) : 197-215/1989.
  10. *Combust. Theor. Model.*, 3(2) : 359-369/1999.
  11. P.A. Boettcher. *Ph.D Thesis. Caltech*, 2012.

# Outline

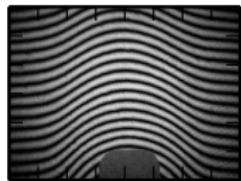
- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

# Current experimental work

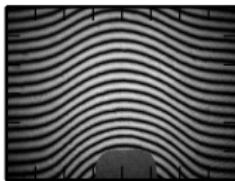
## Ongoing Experimental Efforts at Caltech<sup>12</sup>

**n-Hexane-Air,  $p = 101 \text{ kPa}$ ,  $\Phi = 0.9$ ,  $T_{\text{ign}} = 1175 \text{ K} \pm 40 \text{ K}$**

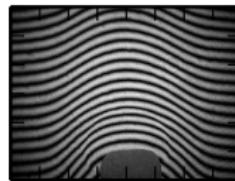
$t = 3.97727 \text{ s}$



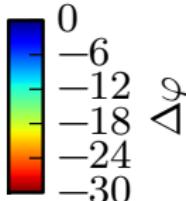
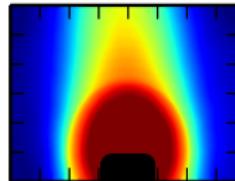
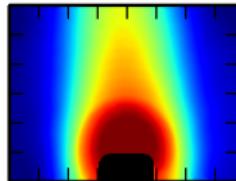
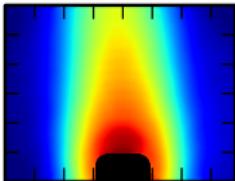
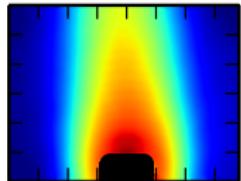
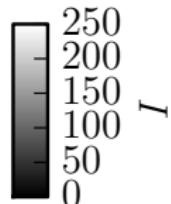
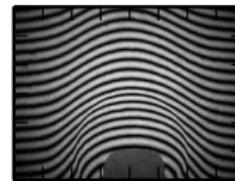
$t = 3.97750 \text{ s}$



$t = 3.97773 \text{ s}$



$t = 3.97781 \text{ s}$



Top : interferometry visualization. Bottom : optical phase difference

12. Courtesy of Augustin Nové-Josserand - Summer intern at EDL (Caltech)

# Outline

- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

# Goal

## Objective

- Explain the dynamics of ignition of combustible gases by transiently heated surfaces - why is ignition more likely to occur at the top ?
- 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

- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

# Physical Model - Governing Equations

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

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

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

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

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

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

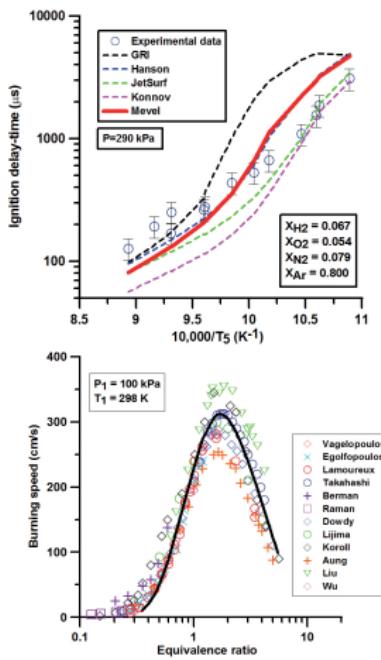
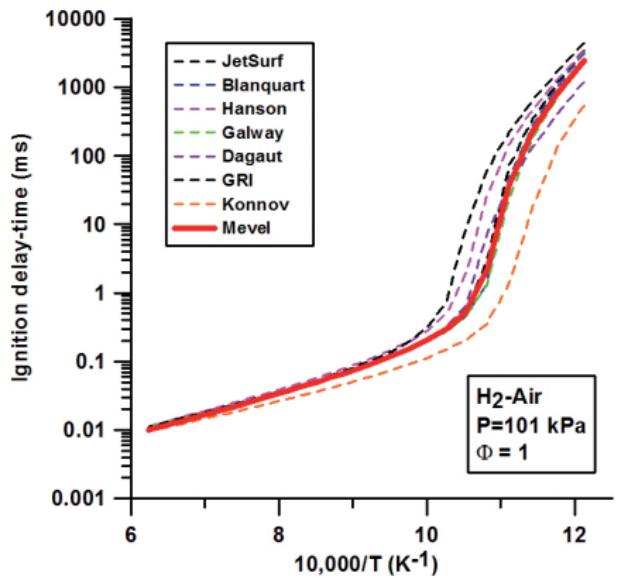
$$h = \sum h_i Y_i, \quad q_{chem} = \sum h_i \Omega_i, \quad \Omega_i = \rho dY_i/dt$$

# Challenges

- Wide range of temporal and spatial scales involved
  - Size of experimental apparatus ( $\mathcal{O}(m)$ )
  - 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 : 2271 reactions and 508 species)

# Physical Model - Hydrogen Chemistry

## Mével's Mechanism (9 species and 21 reactions)<sup>11</sup>



# Approach

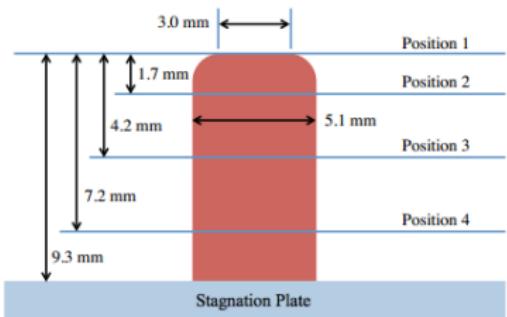
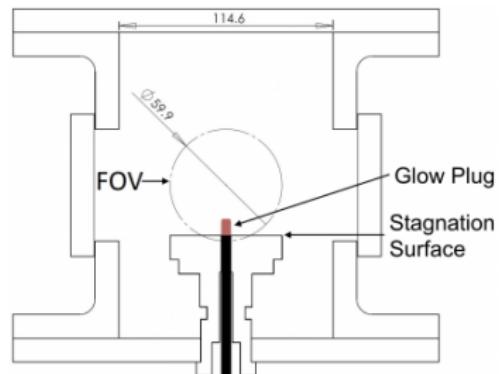
- 2D simulation of reactive viscous flow using the Open source Field Operation And Manipulation (OpenFOAM) toolbox<sup>14</sup>
- Spatial discretization done with Finite Volumes (FV)
- Pressure-velocity coupling achieved using PIMPLE (PISO + SIMPLE)<sup>15</sup>
- Implementation of time dependent boundary 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)

---

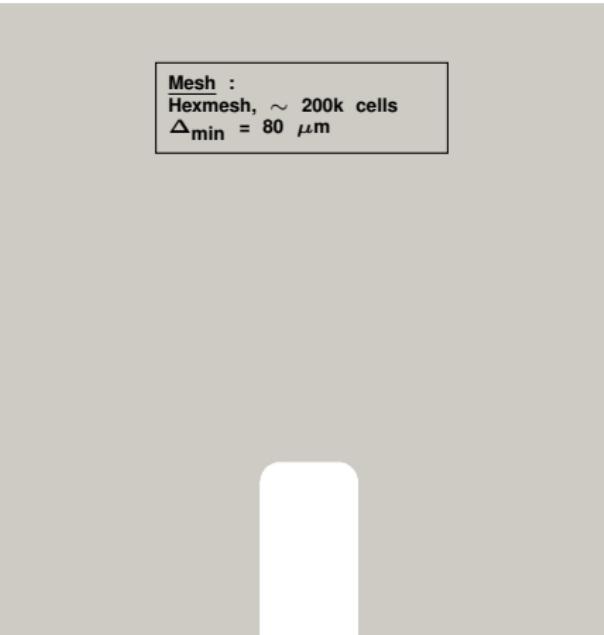
14. H.G. Weller et al. *J. Comput. Phys.*, 12 : 620-631/1998.

15. I. Demirdzic et al. *Int. J. Numer. Meth. Fl.*, 16 : 1029-1050/1993.

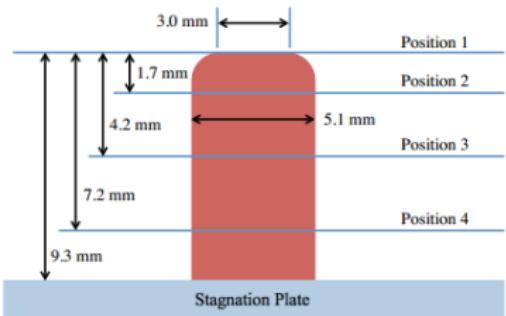
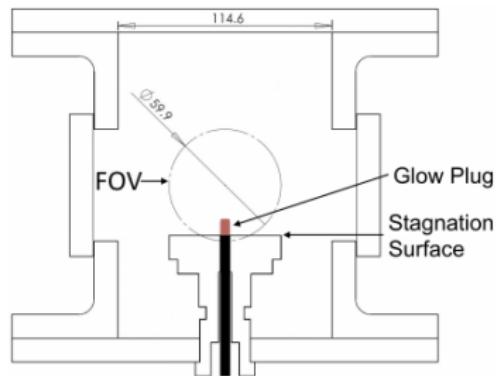
# Experimental setup, initial & boundary conditions



**Mesh :**  
Hexmesh,  $\sim 200k$  cells  
 $\Delta_{\min} = 80 \mu\text{m}$



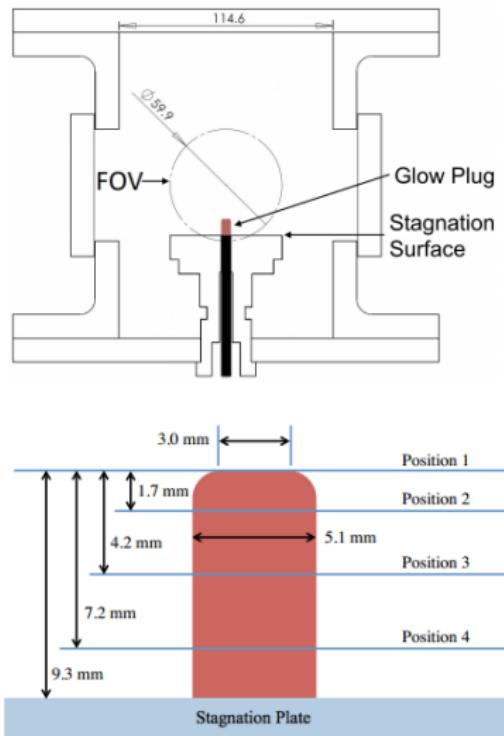
# Experimental setup, initial & boundary conditions



**Mesh :**  
Hexmesh,  $\sim 200k$  cells  
 $\Delta_{\min} = 80 \mu\text{m}$

**Initial Conditions :**  
 $P_0 = 100\text{KPa}$   
 $T_0 = 300\text{K}$   
 $Y_R = 1$

# Experimental setup, initial & boundary conditions

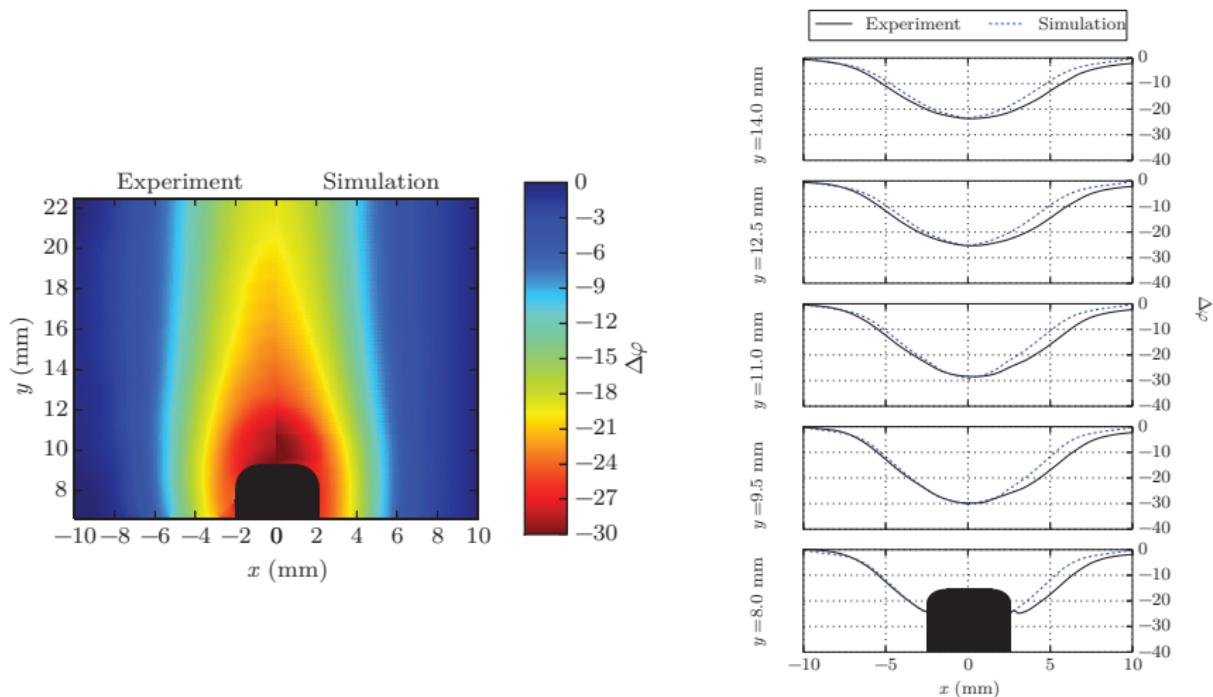


**Mesh :**  
Hexmesh,  $\sim 200k$  cells  
 $\Delta_{\min} = 80 \mu\text{m}$

**Initial Conditions :**  
 $P_0 = 100\text{ kPa}$   
 $T_0 = 300\text{ K}$   
 $Y_R = 1$

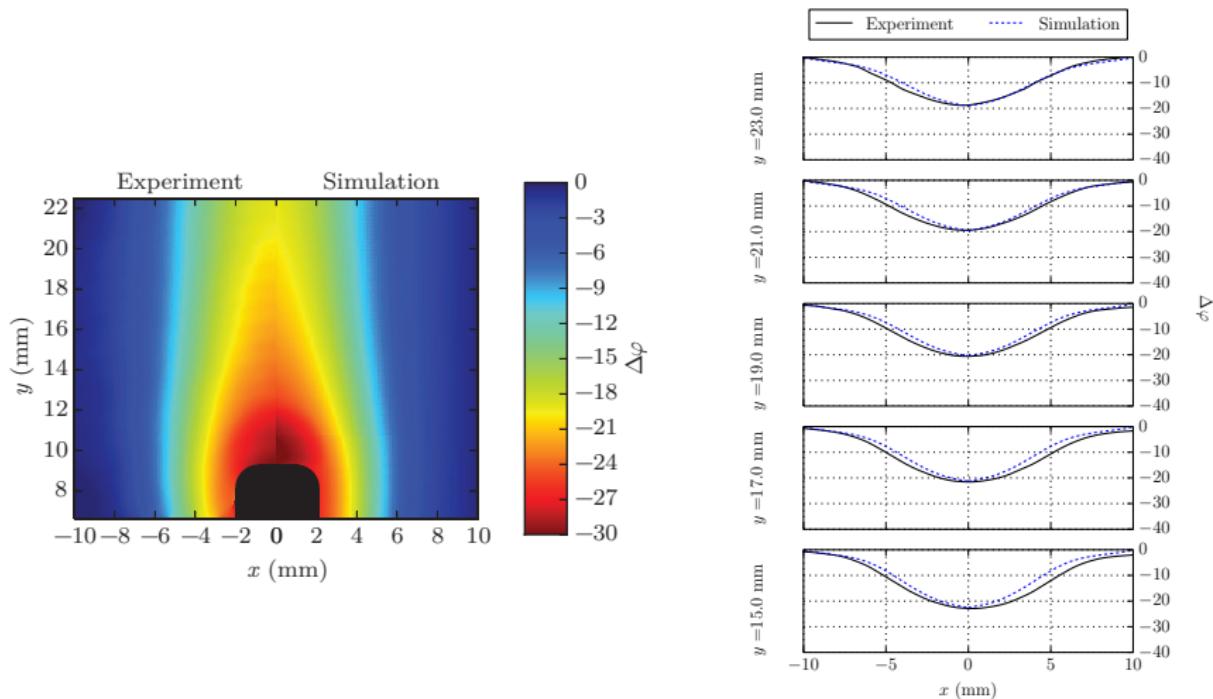
**Boundary Conditions :**  
 $T_w(t) = T_0 + \alpha t$   
 $\alpha$  : heating rate - 220 K/s

# Thermal plume comparison with experiments (1/2)



**Quantitative comparison of experimental (near field) and numerical thermal plume during heating - optical phase difference ( $\Delta\varphi$ ) fields**

# Thermal plume comparison with experiments (2/2)



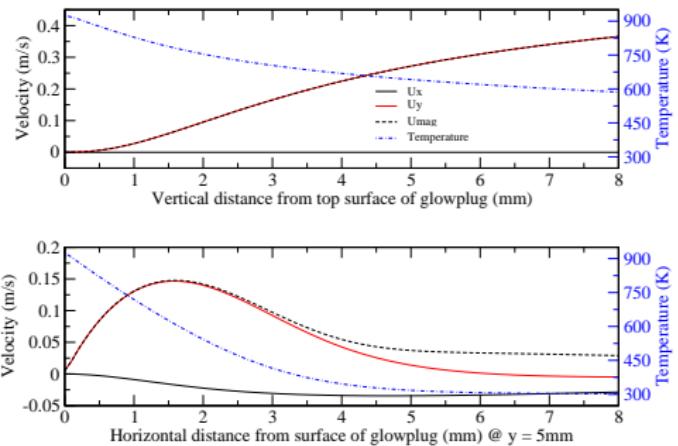
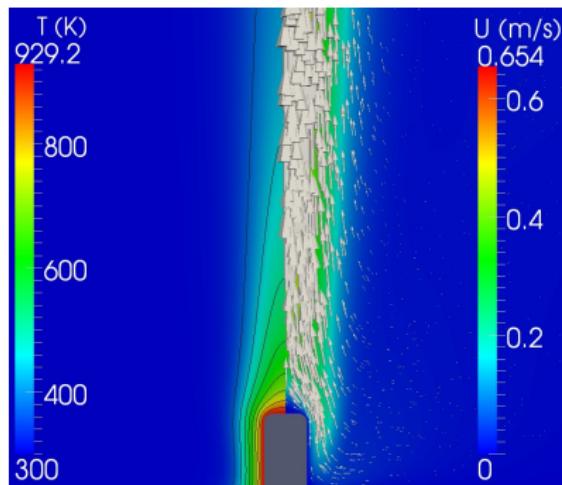
**Quantitative comparison of experimental (far field) and numerical thermal plume during heating - optical phase difference ( $\Delta\varphi$ ) fields**

# Outline

- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

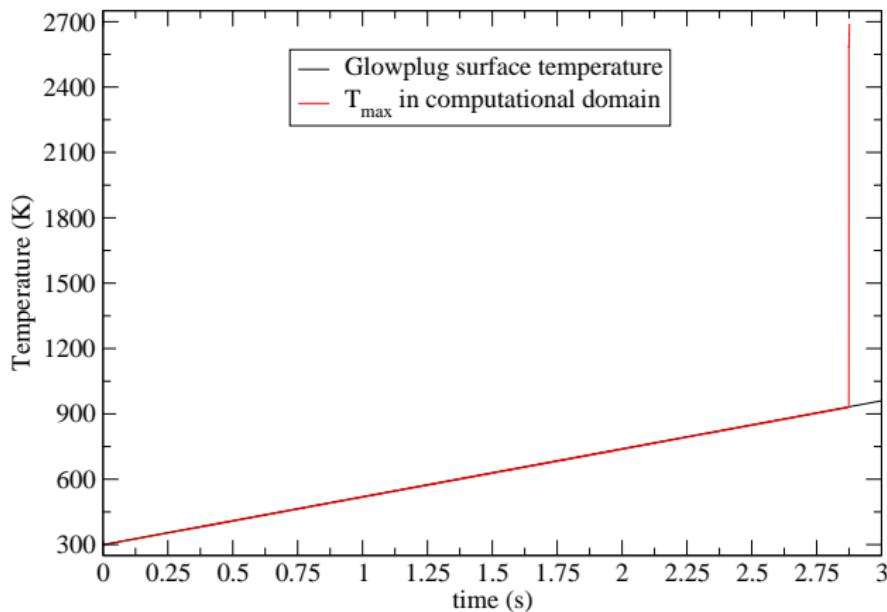
# Flow structure - boundary layer development

$t = 4\text{ s}$



# When does ignition take place ?

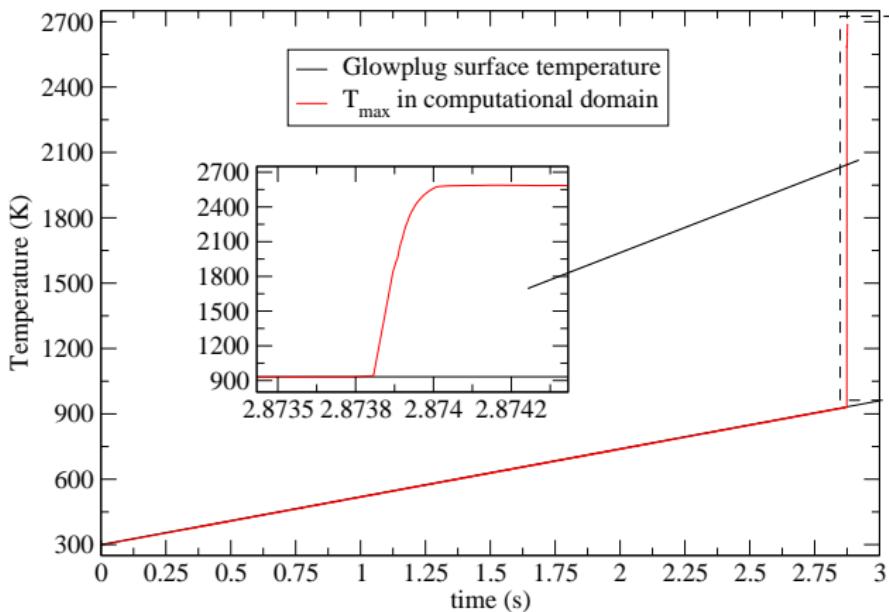
Glowplug - heating rate : 220 K/s



Temperature maximum in computational domain -  $\tau_{\text{ign}} = T_{\text{glow plug}} + 150\text{K}$

# When does ignition take place ?

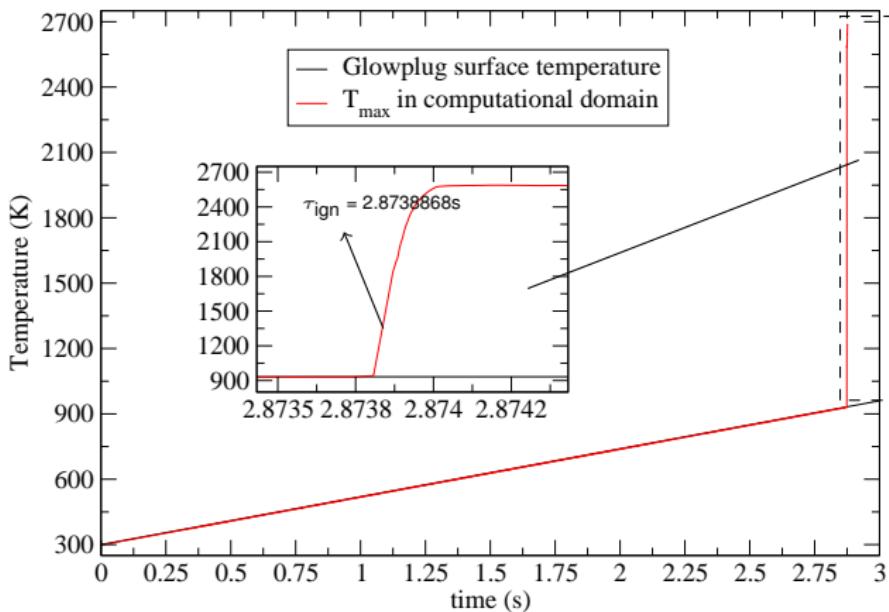
Glowplug - heating rate : 220 K/s



Temperature maximum in computational domain -  $\tau_{\text{ign}} = T_{\text{glow plug}} + 150\text{K}$

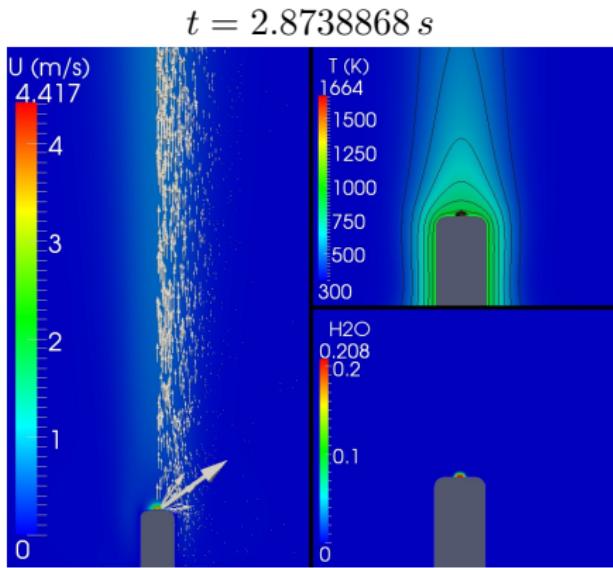
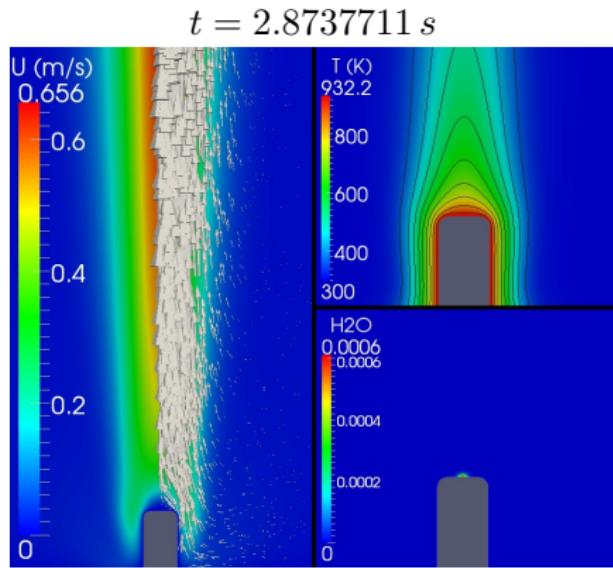
# When does ignition take place ?

Glowplug - heating rate : 220 K/s

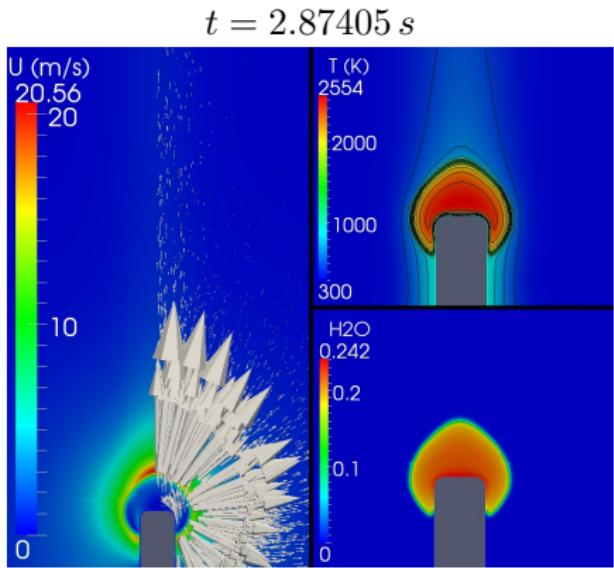
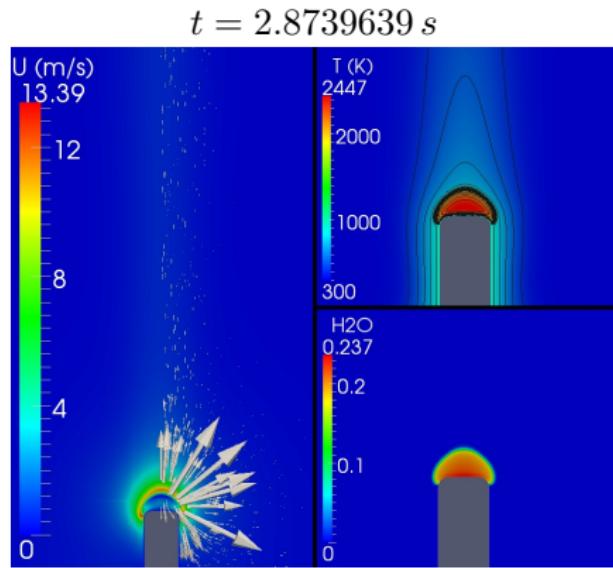


Temperature maximum in computational domain -  $\tau_{\text{ign}} = T_{\text{glow plug}} + 150\text{K}$

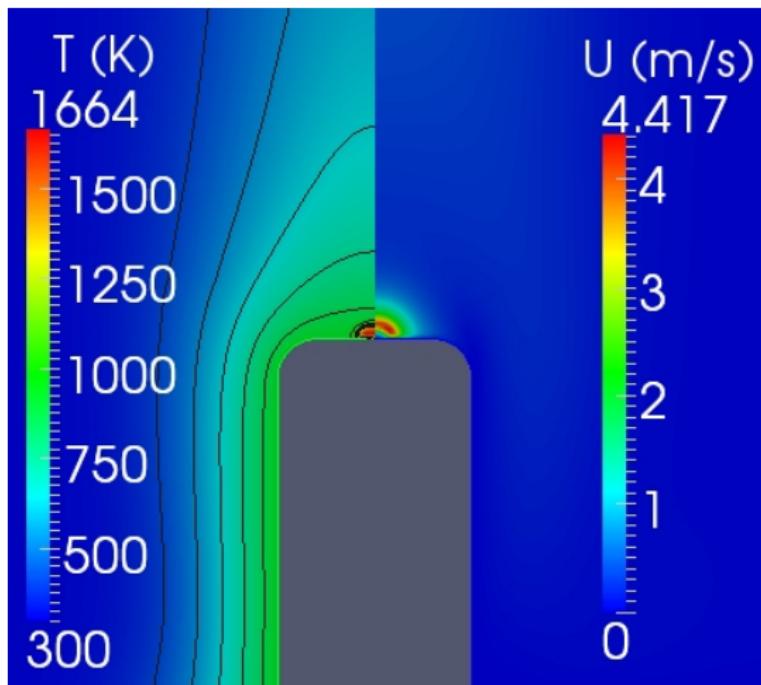
# Where does ignition take place? (1/3)



# Where does ignition take place ? (2/3)



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



Closeup to ignition location

# Outline

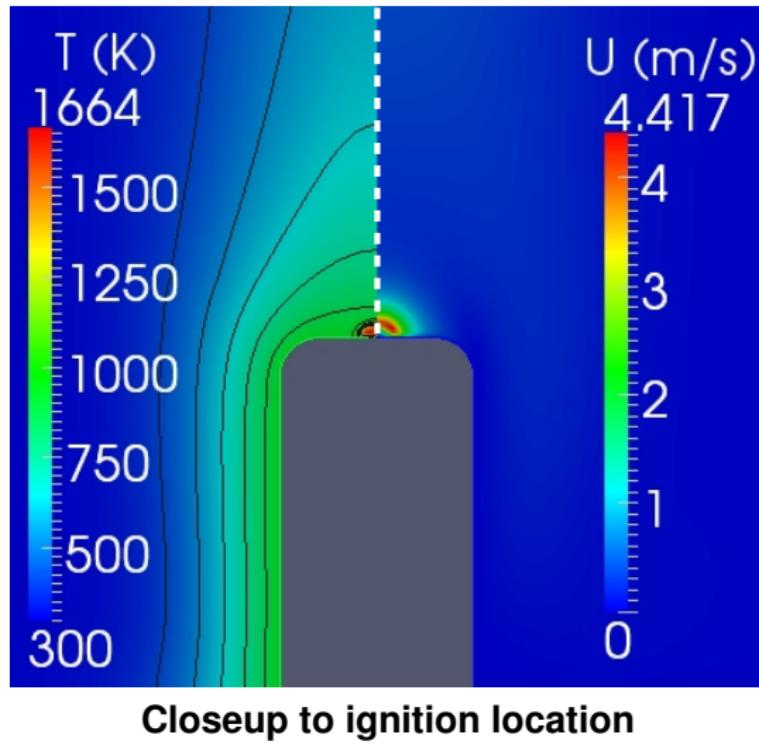
- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

# Energy equation analysis (1/3)

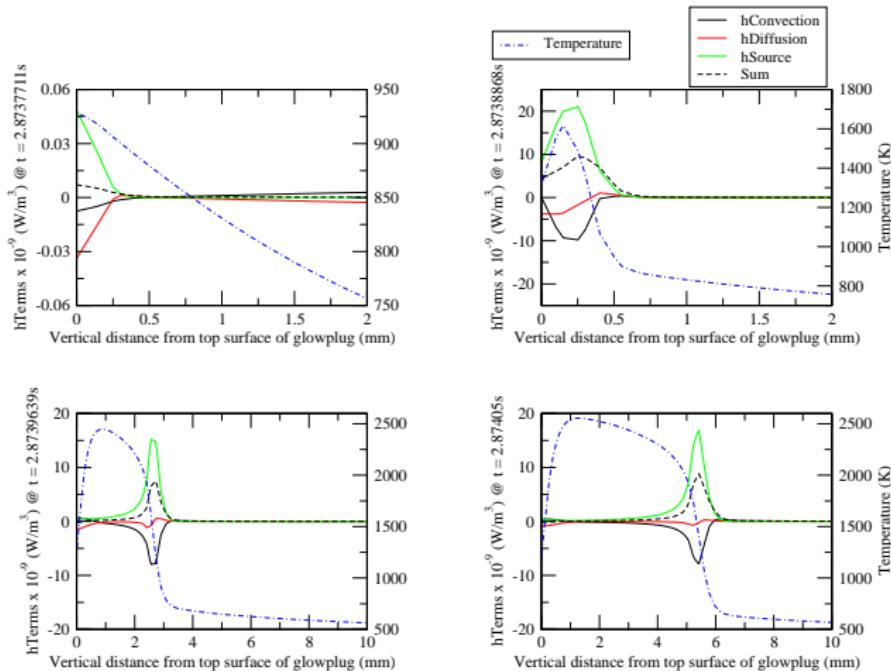
Recall the energy equation

$$\underbrace{\frac{\partial(\rho h)}{\partial t}}_{\text{Sum } (\text{---})} = \underbrace{-\nabla \cdot (\rho \mathbf{u} h)}_{\text{hConvection } (\text{---})} + \underbrace{\nabla \cdot (\kappa/c_p \nabla h)}_{\text{hDiffusion } (\text{---})} + \underbrace{q_c \Omega_R}_{\text{hSource } (\text{---})}$$

# Energy equation analysis (2/3)

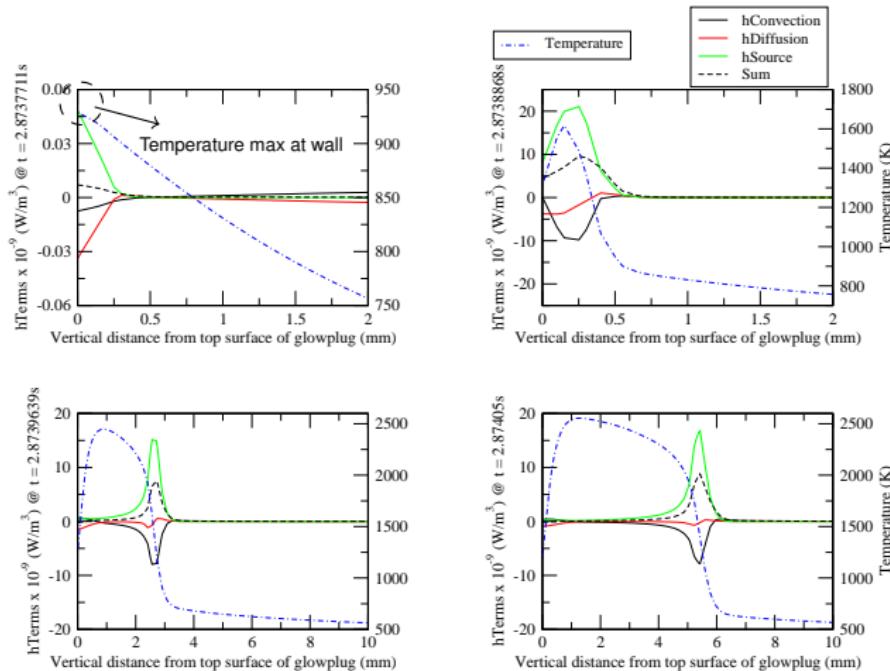


# Energy equation analysis (3/3)



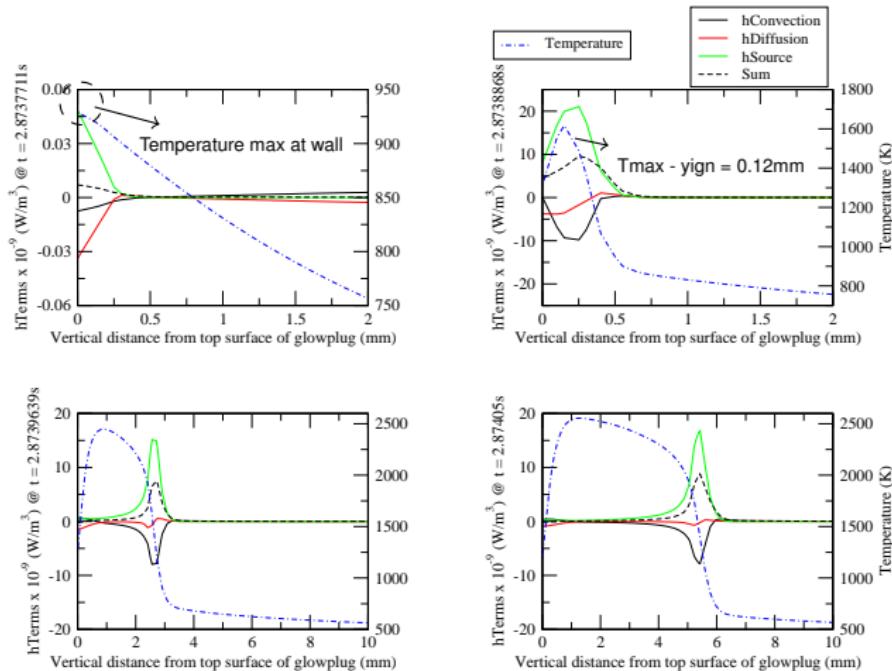
**Contributions of each term in energy equation and temperature along vertical centerline from top of glowplug**

# Energy equation analysis (3/3)



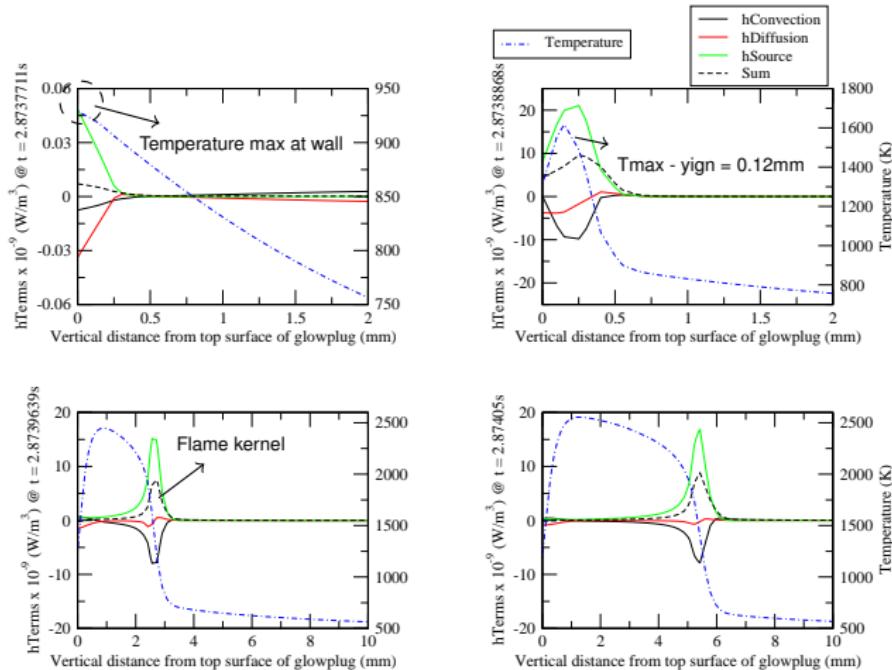
**Contributions of each term in energy equation and temperature along vertical centerline from top of glowplug**

# Energy equation analysis (3/3)



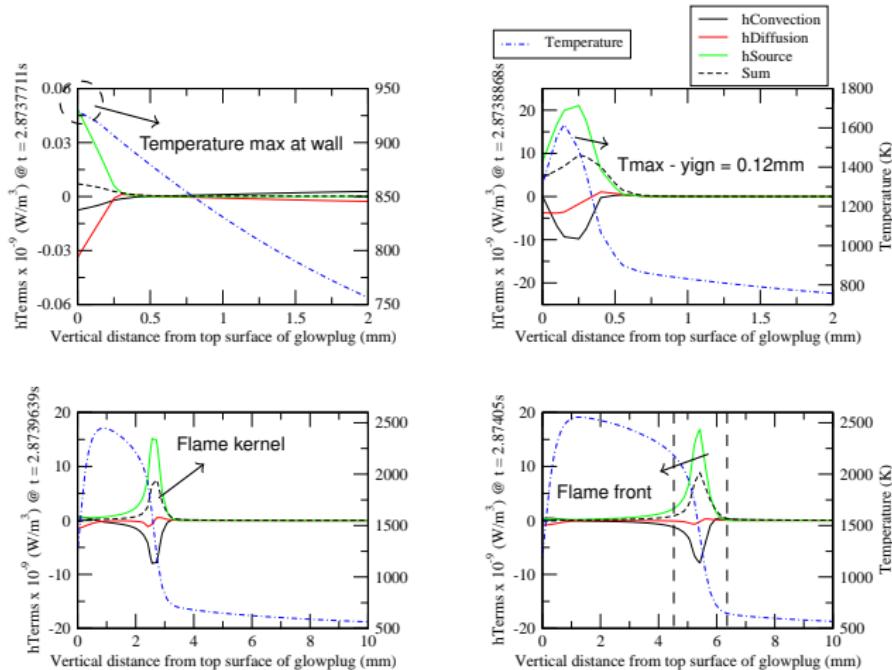
**Contributions of each term in energy equation and temperature along vertical centerline from top of glowplug**

# Energy equation analysis (3/3)



**Contributions of each term in energy equation and temperature along vertical centerline from top of glowplug**

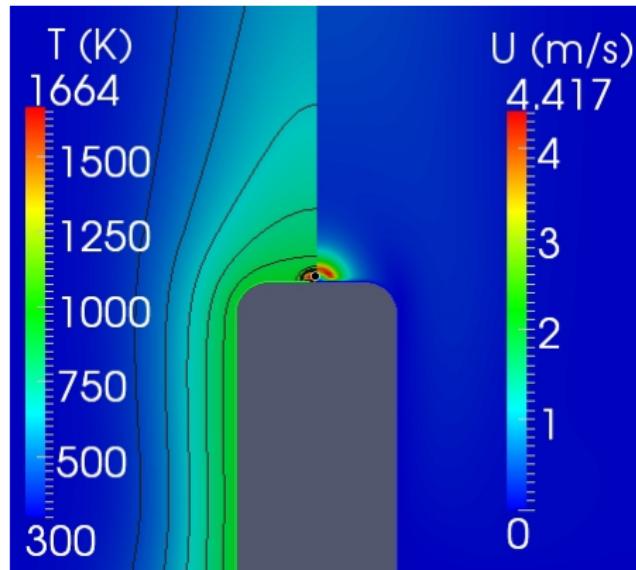
# Energy equation analysis (3/3)



**Contributions of each term in energy equation and temperature along vertical centerline from top of glowplug**

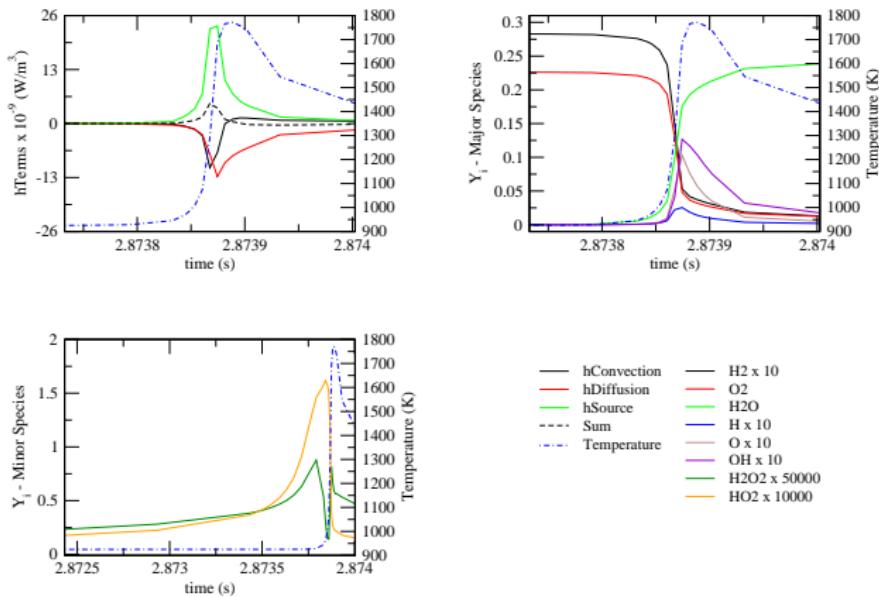
# Temporal evolution near ignition location (1/2)

Glowplug - heating rate = 220 K/s



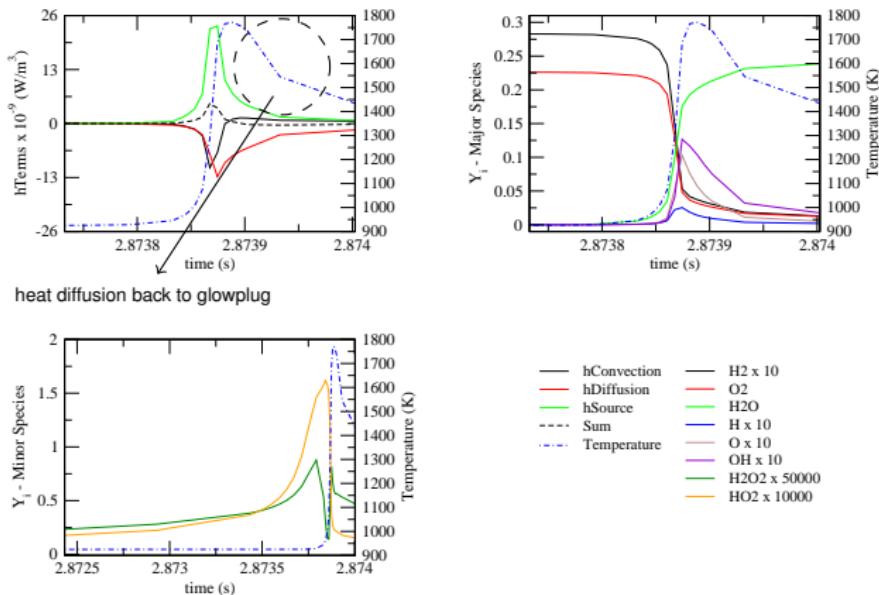
Closeup to ignition location -  $y_{ign} = 0.12 \text{ mm}$

# Temporal evolution near ignition location (2/2)



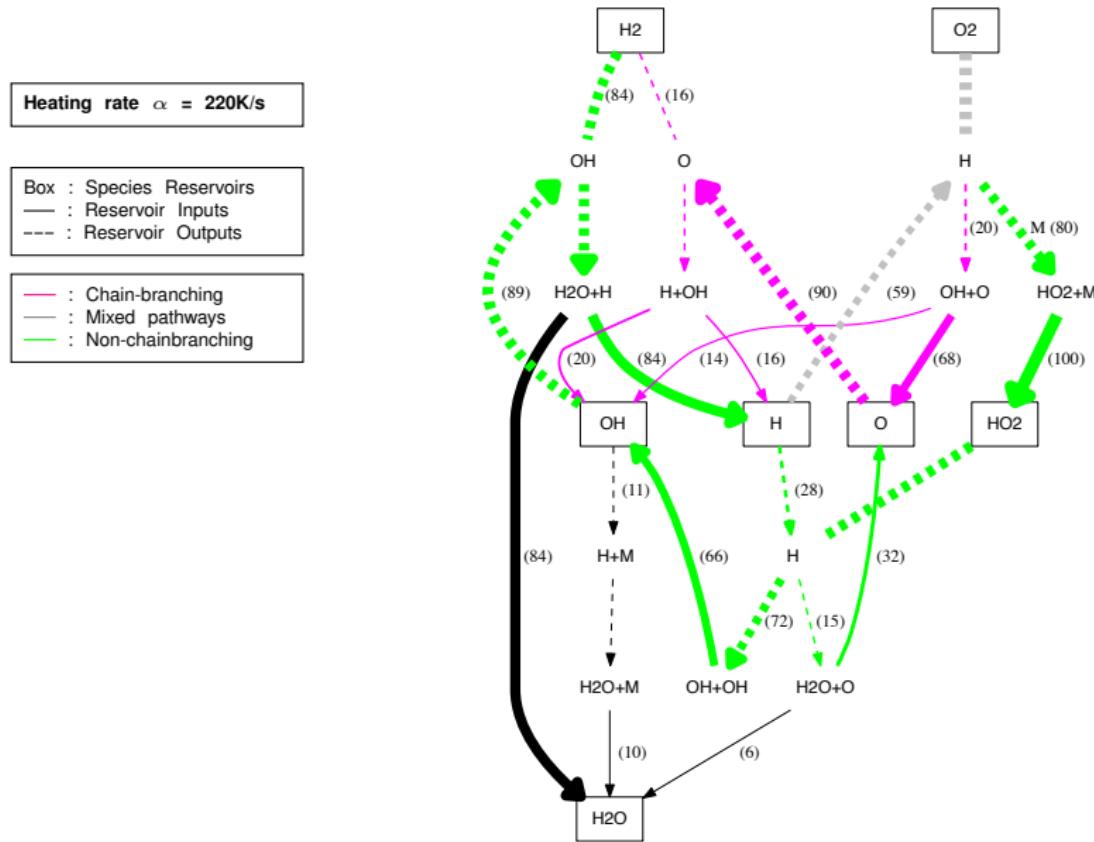
**Temporal Evolution of each term in energy equation, temperature and species mass fractions at the ignition location**

# Temporal evolution near ignition location (2/2)



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

# Chemical Pathways



# Chemical Pathways

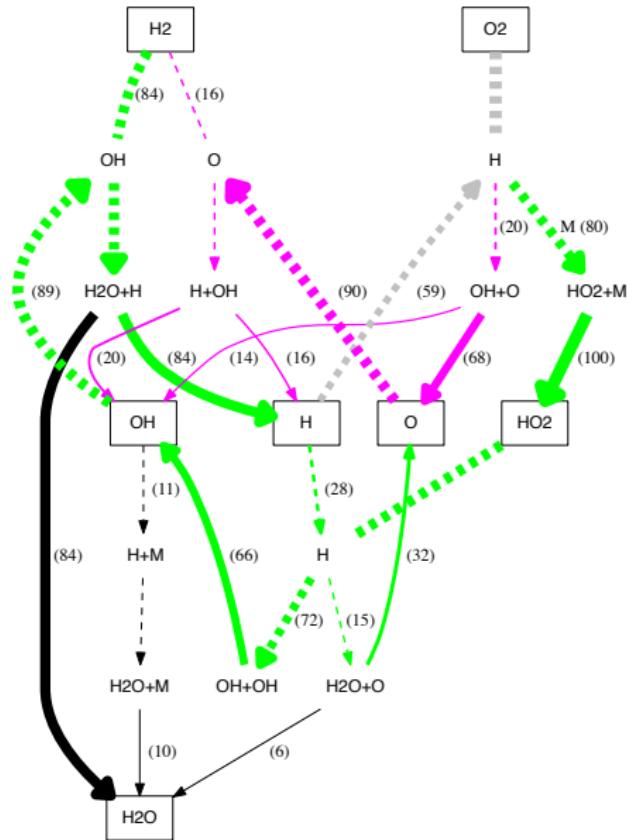
Heating rate  $\alpha = 220\text{K/s}$

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

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

## Chain-branching :

OH radicals produced by chain branching processes (34%)



# Chemical Pathways

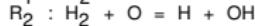
Heating rate  $\alpha = 220\text{K/s}$

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

: Chain-branching  
 : Mixed pathways  
 : Non-chainbranching

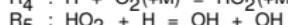
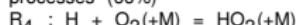
## Chain-branching :

OH radicals produced by chain branching processes (34%)

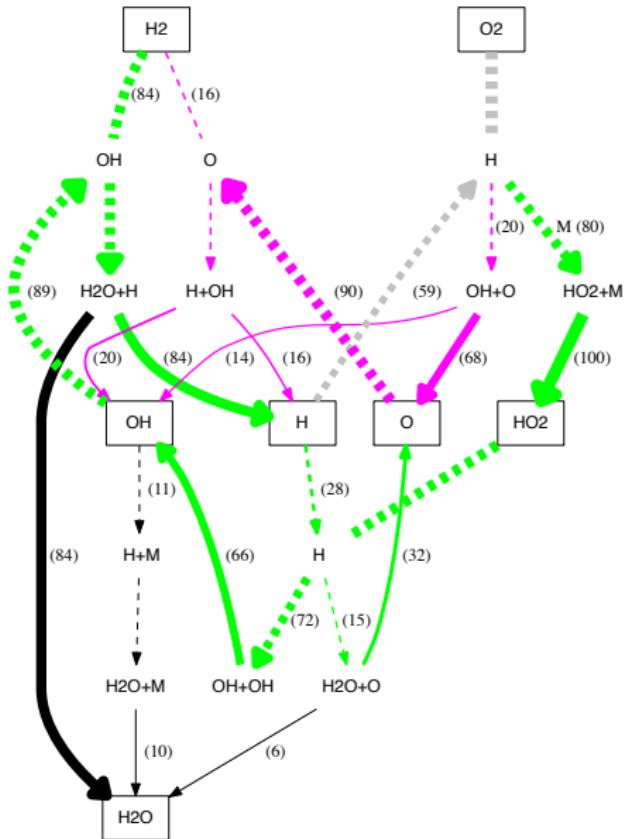


## Non-chain branching :

OH radicals produced by non-chain branching processes (66%)



Dominant pathway - Impact of low temperature chemistry in ignition process

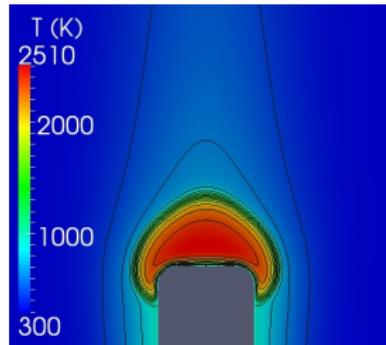
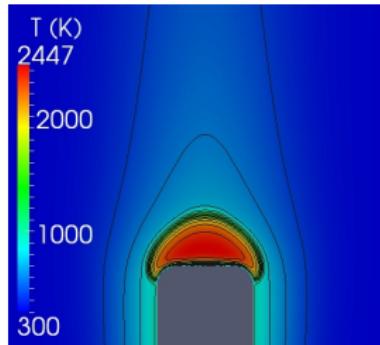
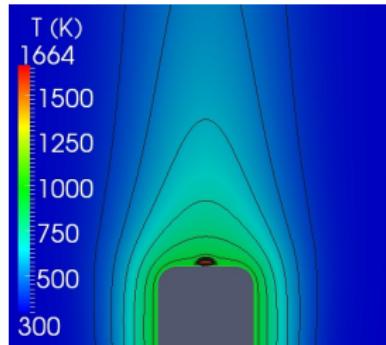


# Outline

- 1 Motivation
- 2 Previous Work
- 3 Current Experimental Work
- 4 Goal
- 5 Physical Model, Numerical Approach and Simulation Parameters
- 6 Results
- 7 Discussion
- 8 Closing Remarks

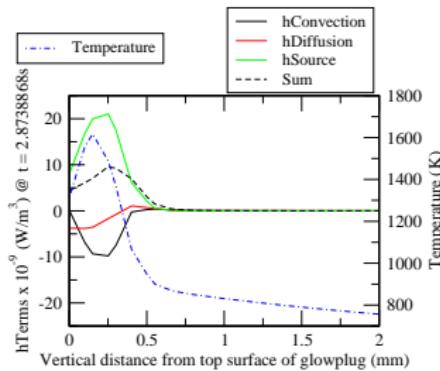
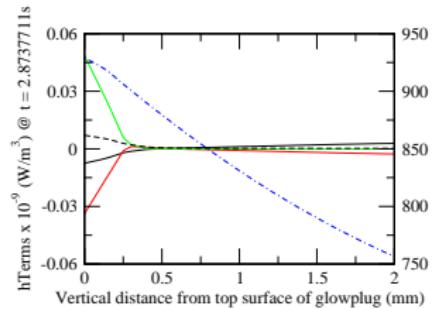
# Closing Remarks (1/3)

- In good agreement with experiments, ignition was observed to occur at the top of the glowplug



# Closing Remarks (2/3)

- Boundary layer separation plays a crucial role in creating zones that are prone to ignition
  - convective transport of energy and species out of the separated region is minimized, and the build up of species and energy can only be opposed by diffusion, facilitating the thermal runaway that characterizes ignition



# Closing Remarks (3/3)

- 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

# Conclusion

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

