

# Effect of rotation on ignition thresholds of stoichiometric hydrogen-air mixtures

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**Caltech**

# Outline

1 Motivation

2 Background and previous work

3 Goal

4 Computational methodology

5 Results

6 Closing remarks

# The big picture - motivation

**How can we mitigate/prevent accidental combustion events in industries where a single accident can lead to large scale destruction + losses of lives + environmental impact ?**



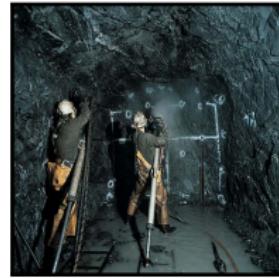
Aircraft



Nuclear



Chemical



Mining

# The big picture - motivation

**How can we mitigate/prevent accidental combustion events in industries where a single accident can lead to large scale destruction + losses of lives + environmental impact ?**



Aircraft



Nuclear



Chemical



Mining

through improved/fundamental understanding of ignition hazards

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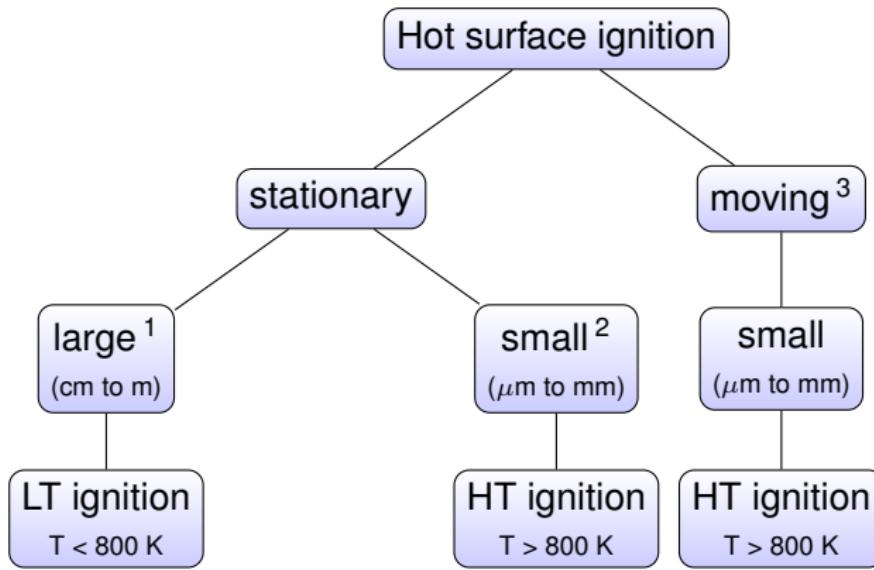
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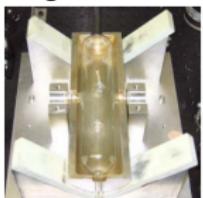
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# Background - characterization of hot surface ignition

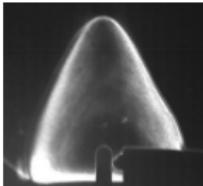
How can thermal ignition occur ? fuel + oxidizer + ign. source



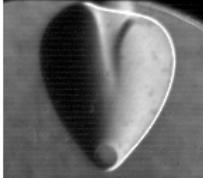
Large & stationary



Small & stationary



Moving & small



1. Kutcha (1965), Council (1983), Colwell & Reza (2005), **Melguizo-Gavilanes et al. (2016)**

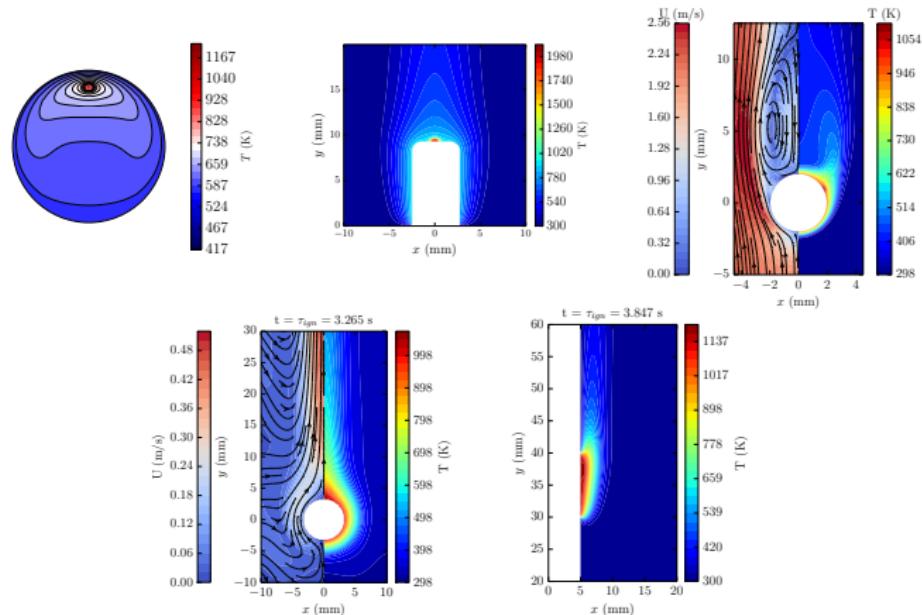
2. Smyth & Bryner (1997), Dubaniewicz (2000, 2003, 2006), Beyer & Markus (2012), Roth et al. (2014), Boettcher (2012), **Melguizo-Gavilanes et al. (2016)**, Menon et al. (2016)

3. Silver (1937), Paterson (1939, 1940), Coronel (2016), **Melguizo-Gavilanes et al. (2016)**

# Previous work - main learnings

## Key results

- ✓ Critical conditions for ignition arise in regions where temperature gradients are small through competition between chemical reaction and transport processes
- ✓ Results suggest this is a universal feature of both natural and forced convection in internal and external flows



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# Goal

## Question

- ✓ Does rotation of a hot surface affect the ignition threshold of a stoichiometric fuel-air mixture ?

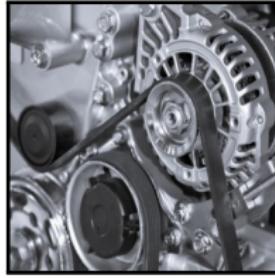
# Goal

## Question

- ✓ Does rotation of a hot surface affect the ignition threshold of a stoichiometric fuel-air mixture ?

## Why ?

- ✓ Hot shafts present in industrial settings and could pose an ignition hazard ...



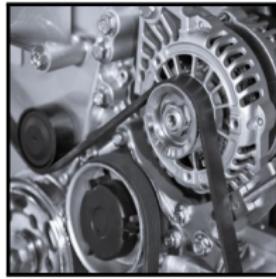
# Goal

## Question

- ✓ Does rotation of a hot surface affect the ignition threshold of a stoichiometric fuel-air mixture ?

## Why ?

- ✓ Hot shafts present in industrial settings and could pose an ignition hazard ...



## Plan of attack

- ✓ Numerically asses the effect of rotation on reported ignition thresholds using horizontal cylinders rotating at different angular velocities

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# Governing equations

Reactive Navier-Stokes with temperature dependent properties

$$\partial_t(\rho) + \nabla \cdot (\rho \vec{u}) = 0$$

$$\partial_t(\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot \tau + \rho \vec{g}$$

$$\partial_t(\rho Y_i) + \nabla \cdot (\rho \vec{u} Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{\omega}_i, \quad Le_i = \kappa / (c_p \rho D_i)$$

$$\partial_t(\rho h_s) + \nabla \cdot (\rho \vec{u} h_s) = \nabla \cdot \left\{ \frac{\kappa}{c_p} \nabla h_s - \sum_{i=1}^N h_{s,i} (1 - 1/Le_i) \frac{\kappa}{c_p} \nabla Y_i \right\} + \dot{q}_{chem}$$

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

$$h_s = \int_{T_o}^T \left( \sum_{i=1}^N c_{p,i} Y_i \right) dT, \quad \dot{q}_{chem} = - \sum_{i=1}^N \Delta h_{f,i}^o \dot{\omega}_i$$

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# Transport models

- ✓ Two coefficient ( $A_s$  and  $T_s$ ) Sutherland law for mixture viscosity<sup>4</sup> - optimized using Cantera for temperature range of interest (300-2500 K)

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4. W. Sutherland (1893), Philos. Mag. Ser. 5 36 507–531.
  5. B. Poling, J. Prausnitz, J. O'Connell, The Properties of Gases and Liquids, 2000.
  6. A. Burcat, R. Branko, Argonne National Laboratory (ANL), July 29, 2005.
  7. T. Poinsot, D. Veynante, Theoretical and Numerical Combustion, Edwards, Philadelphia PA, USA, 2005.

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- ✓ Constant, non-unity Le specified for each species<sup>7</sup> - species diffusivities computed using Cantera

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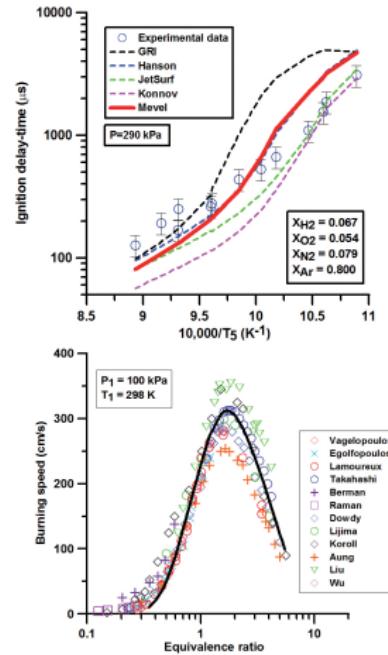
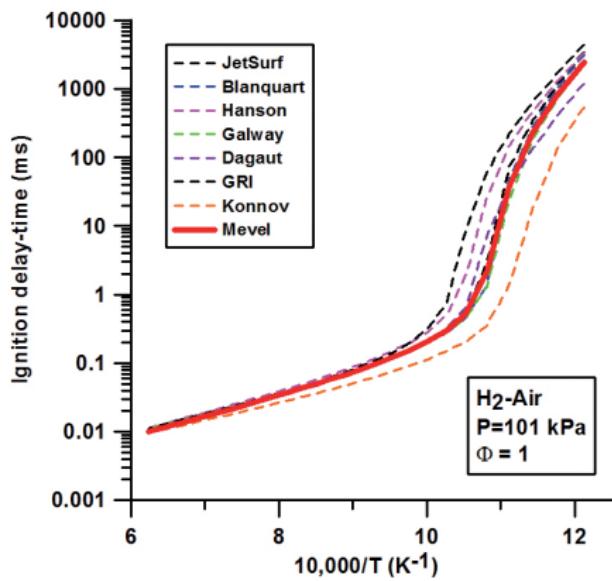
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7. T. Poinsot, D. Veynante, Theoretical and Numerical Combustion, Edwards, Philadelphia PA, USA, 2005.

# Chemical model - hydrogen chemistry

## Mével's Mechanism (9 species and 21 reactions)<sup>8</sup>



8. R. Mével et al. (2009, 2011) *P. Combust. Inst.*, 32 & 33

# Approach

- ✓ 2D simulations of reactive viscous flow using the Open source Field Operation And Manipulation (OpenFOAM) toolbox<sup>9</sup>
- ✓ Spatial discretization done with Finite Volumes (FV)
- ✓ Pressure-velocity coupling achieved using PIMPLE (PISO + SIMPLE)<sup>10</sup>
- ✓ Implementation of differential diffusion and 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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9. H.G. Weller et al. (1998) *J. Comput. Phys.*, 12 : 620-631.

10. I. Demirdzic et al. (1993) *Int. J. Numer. Meth. Fl.*, 16 : 1029-1050.

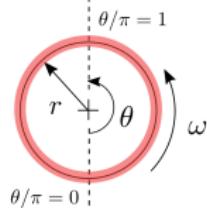
# Domain, initial & boundary conditions

## 2D-planar hexamesh

109,000 cells

$$\Delta_{min} = 40 \mu\text{m}$$

$$r = 5 \text{ mm}$$



## Initial conditions

$$p_o = 100 \text{ kPa}$$

$$T_o = 300 \text{ K}$$

$$U_o = (0,0) \text{ m/s}$$

$$Y_{H2} = 0.0283, Y_{O2} = 0.2264, Y_{N2} = 0.7453$$

## Boundary Conditions

$$T_{surf}(t) = 300 \text{ K} + \alpha t$$

with  $\alpha = 220 \text{ K/s}$

$$\omega = 60, 120, 240, 480 \text{ rad/s}$$

## Boundaries location

Left/right:  $\sim 11.5r$

Top/bottom:  $\sim 15.5r$

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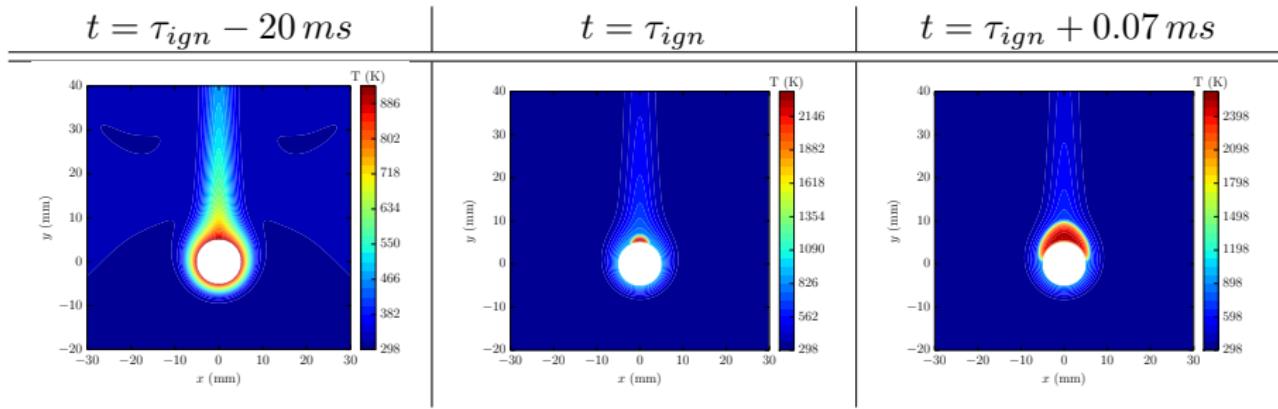
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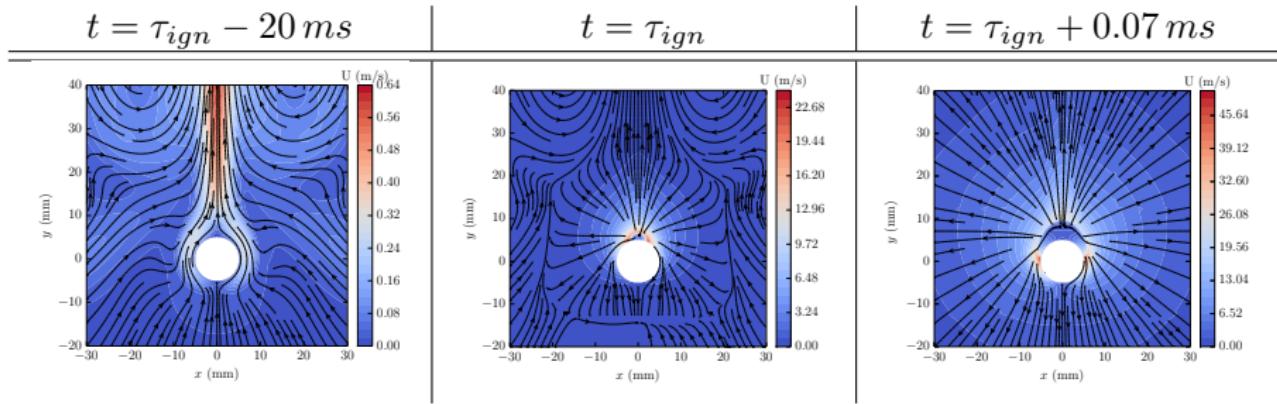
# Flow field and ignition evolution - $\omega = 0$ rad/s (ref. case)

Temperature (K)



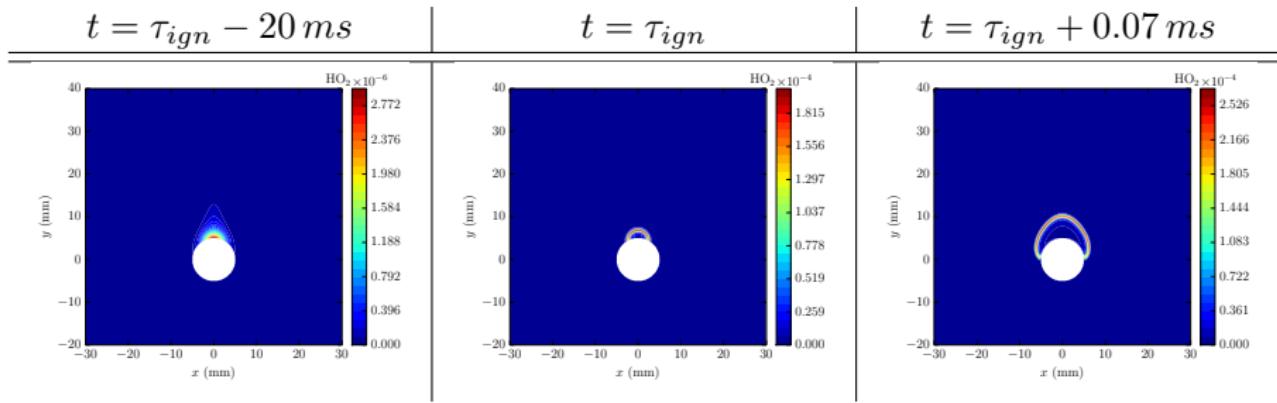
# Flow field and ignition evolution - $\omega = 0$ rad/s (ref. case)

Magnitude of velocity (m/s)



# Flow field and ignition evolution - $\omega = 0$ rad/s (ref. case)

## Mass fraction of HO<sub>2</sub>



# Rationale for choosing $\omega$

The maximum plume velocity before ignition in the reference case,  $U_{p,\max} @ \text{ign}$  ( $\sim 0.6 \text{ m/s}$ ) is used to find relevant values of  $\omega$  to test

$$U_t = r\omega, \quad \omega = U_t/r$$

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$U_t$	$\omega (\text{rad/s})$
$0.5U_{p,\text{max}} @ \text{ign}$	60
$U_{p,\text{max}} @ \text{ign}$	120
$2U_{p,\text{max}} @ \text{ign}$	240
$4U_{p,\text{max}} @ \text{ign}$	480

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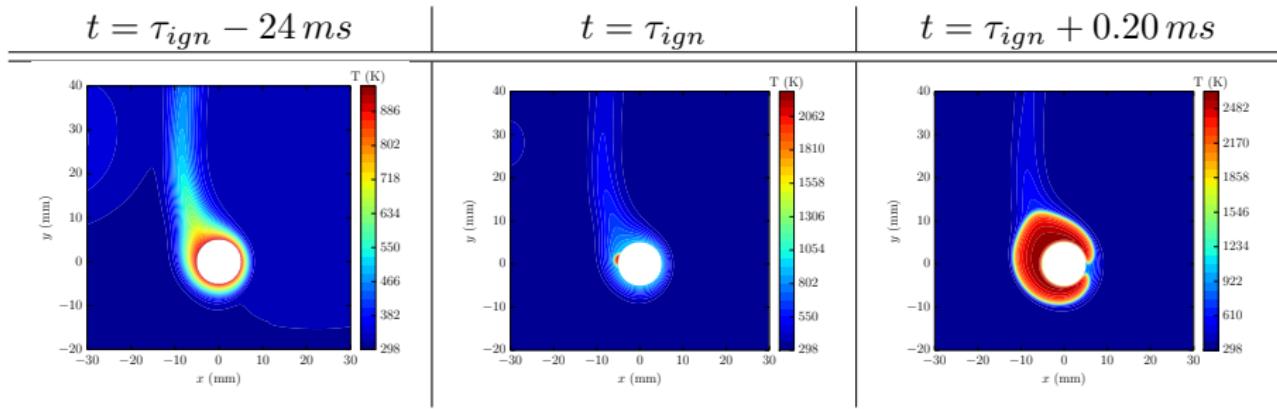
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$U_t$	$\omega (\text{rad/s})$
$0.5U_{p,\text{max}} @ \text{ign}$	60 <span style="color:red">X</span>
$U_{p,\text{max}} @ \text{ign}$	120 <span style="color:green">✓</span>
$2U_{p,\text{max}} @ \text{ign}$	240 <span style="color:green">✓</span>
$4U_{p,\text{max}} @ \text{ign}$	480 <span style="color:green">✓</span>

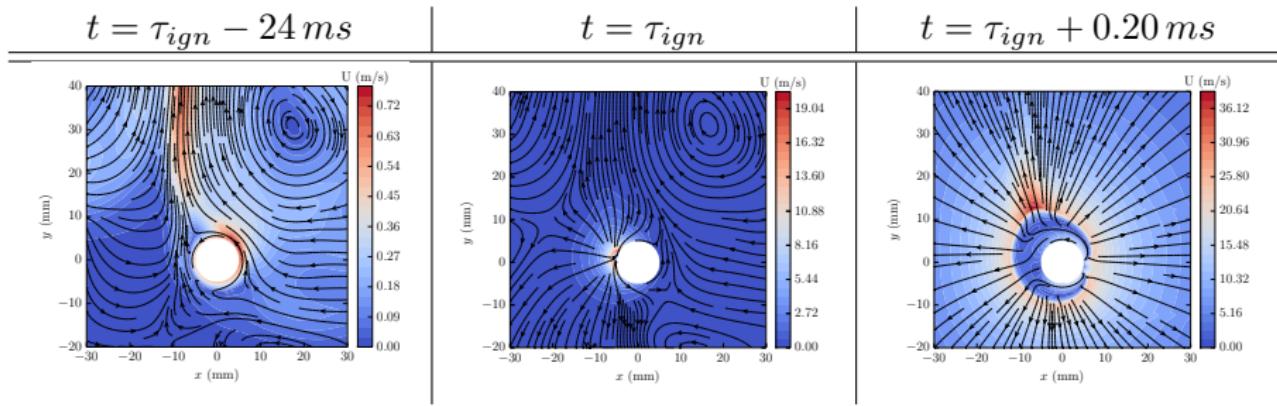
# Flow field and ignition evolution - $\omega = 120 \text{ rad/s}$

Temperature (K)



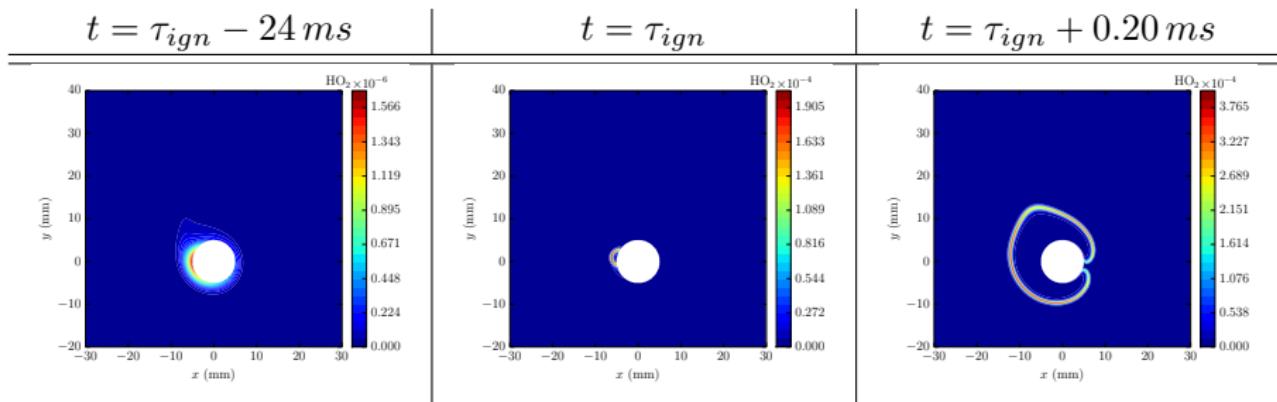
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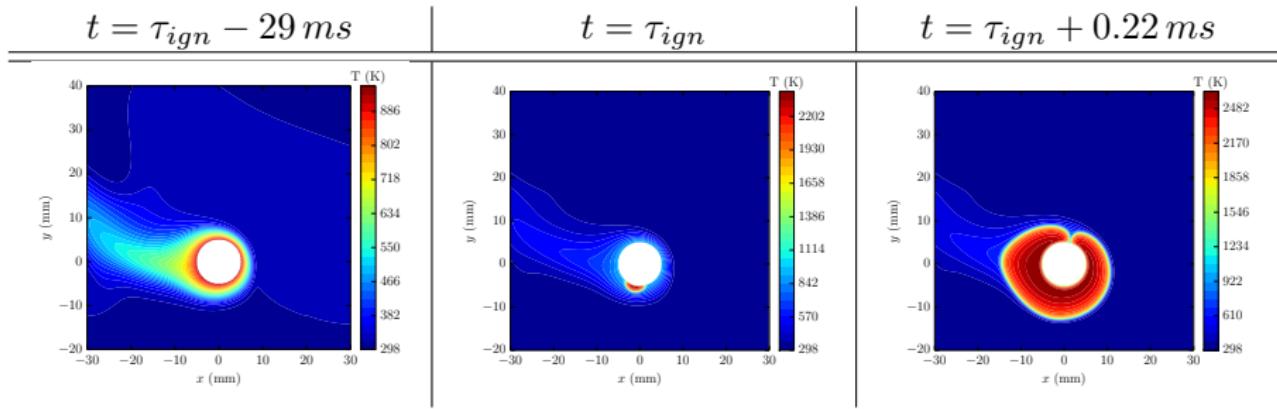
# Flow field and ignition evolution - $\omega = 120 \text{ rad/s}$

## Mass fraction of HO<sub>2</sub>



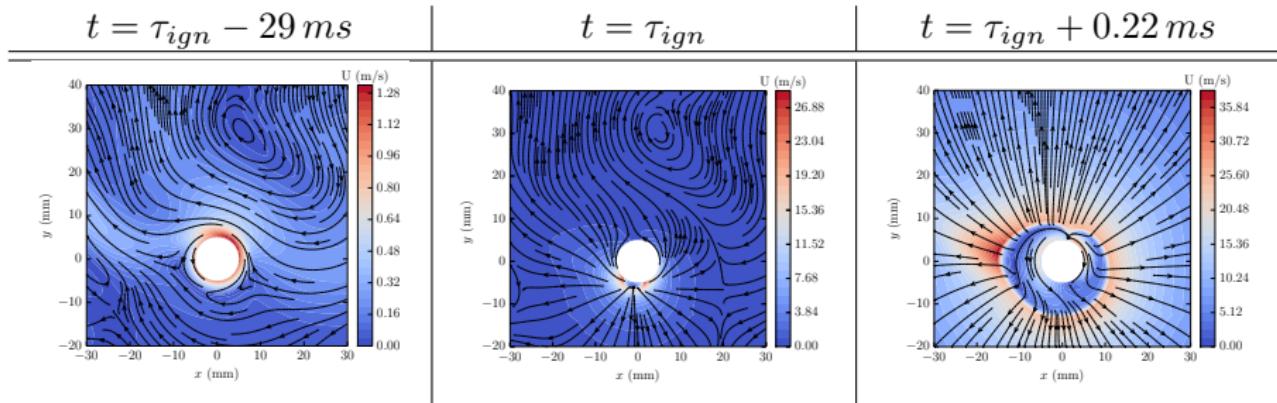
# Flow field and ignition evolution - $\omega = 240 \text{ rad/s}$

Temperature (K)



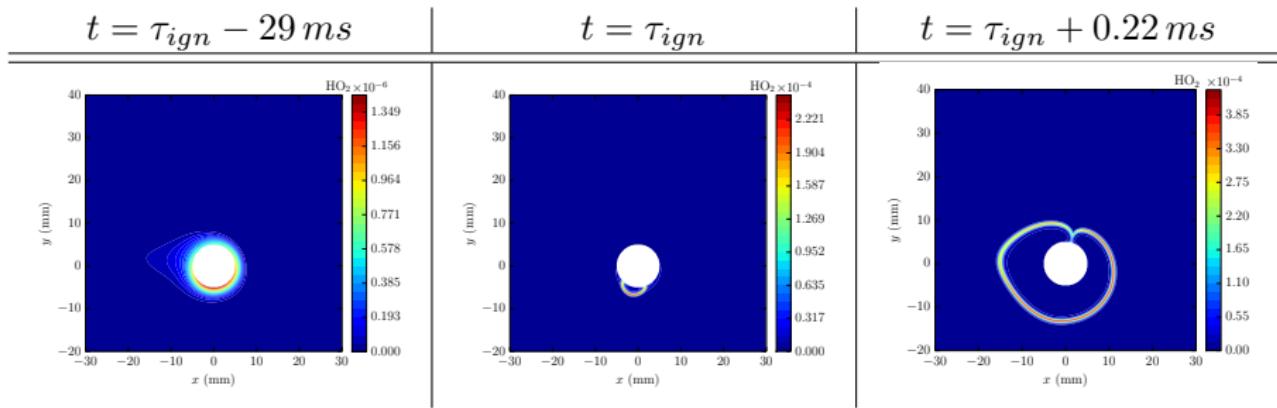
# Flow field and ignition evolution - $\omega = 240 \text{ rad/s}$

Magnitude of velocity (m/s)



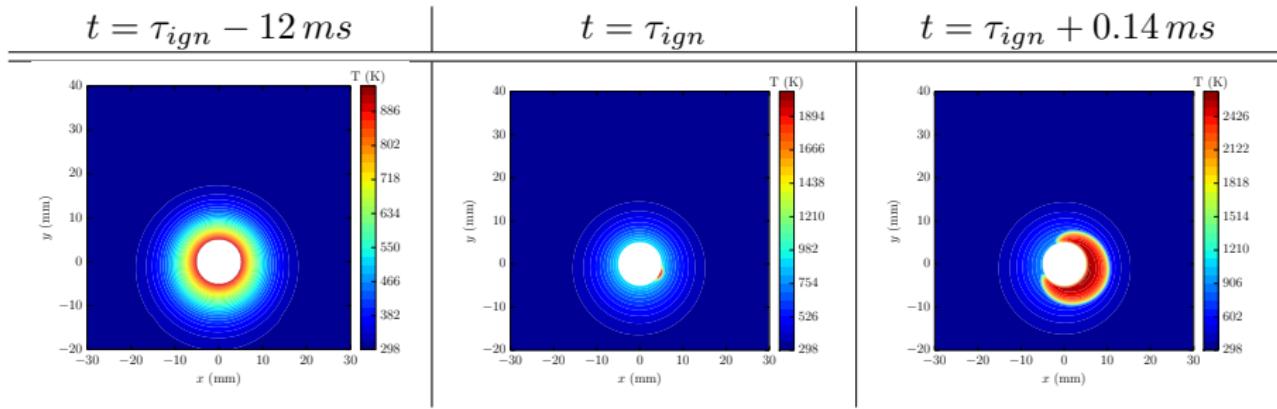
# Flow field and ignition evolution - $\omega = 240 \text{ rad/s}$

## Mass fraction of HO<sub>2</sub>



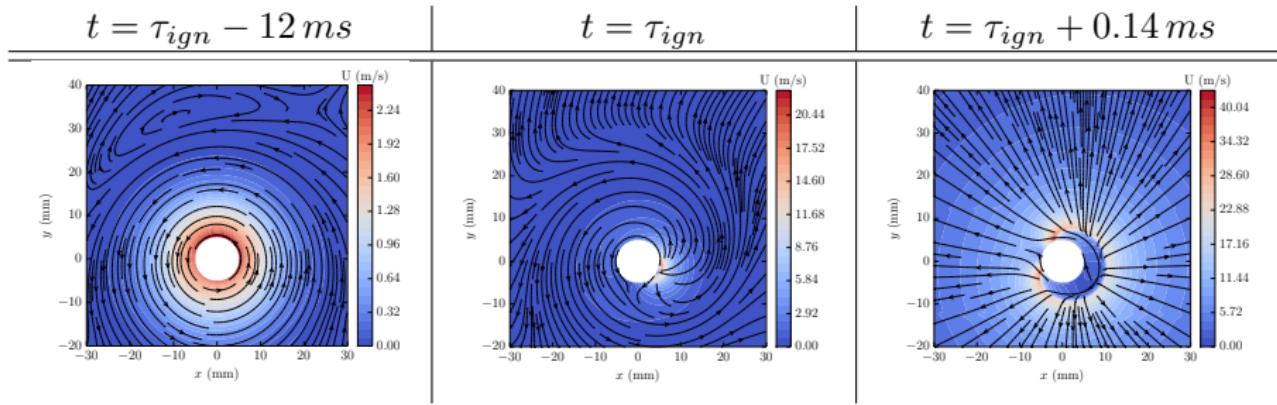
# Flow field and ignition evolution - $\omega = 480 \text{ rad/s}$

Temperature (K)



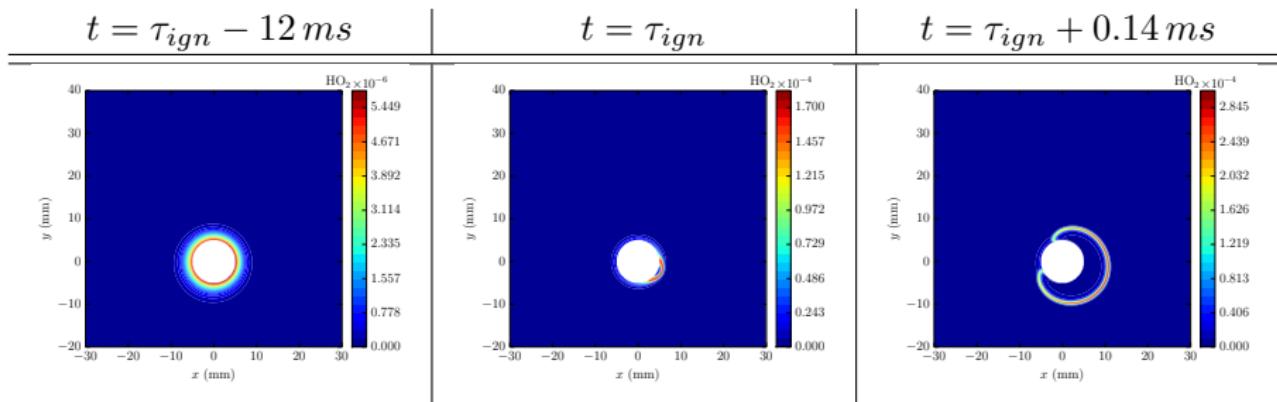
# Flow field and ignition evolution - $\omega = 480 \text{ rad/s}$

Magnitude of velocity (m/s)

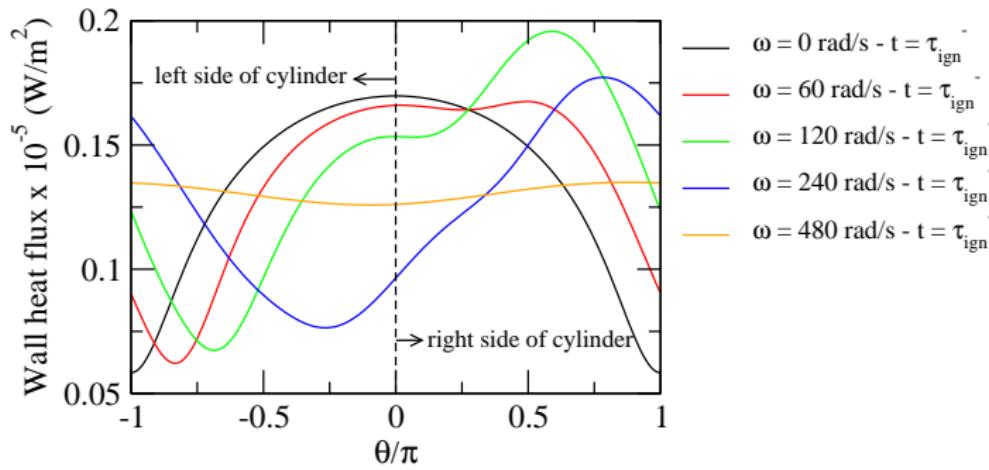


# Flow field and ignition evolution - $\omega = 480 \text{ rad/s}$

## Mass fraction of HO<sub>2</sub>

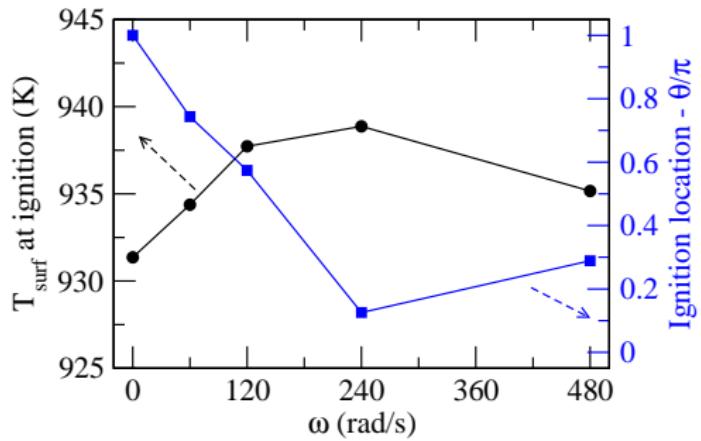


# Wall heat flux along cylinder



**Wall heat flux along heated surface shortly before ignition**

# Predicted ignition thresholds and ignition location



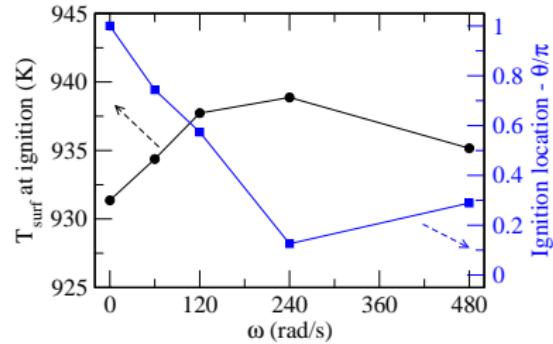
**$T_{surf}$  at ignition and  $\theta/\pi$  as a function of angular velocity**

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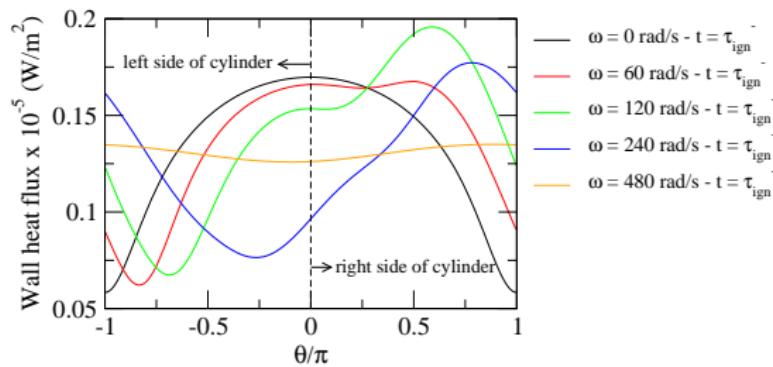
# Closing remarks (1/4)

- ✓ First time a 2D numerical simulation with detailed chemistry is performed to investigate the effect of rotation on the reported ignition thresholds
- ✓ Ignition thresholds for stoichiometric hydrogen-air essentially unaffected by imposing a rotating boundary condition at the surface of the cylinder
- ✓ The location of ignition along the surface of the cylinder showed a stronger variation as a function of angular velocity



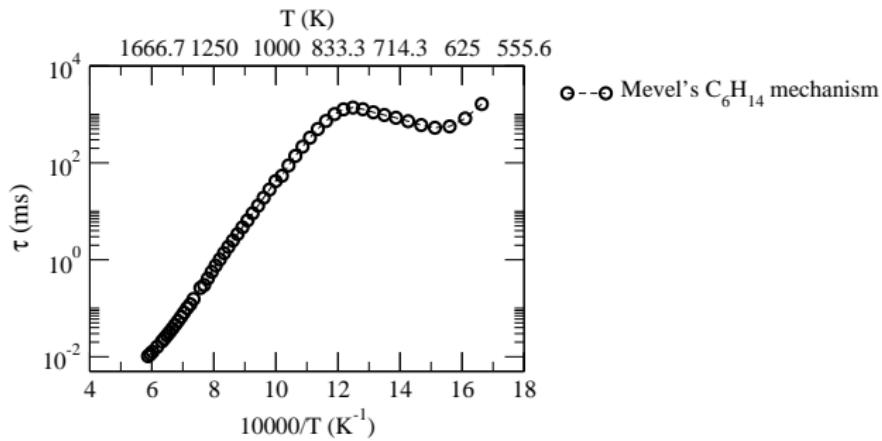
# Closing remarks (2/4)

- ✓ A wall heat flux analysis along the surface of the cylinder revealed the regions that are more likely to ignite : those with shallow temperature gradients (low wall heat flux) as higher temperatures are reached further away from the cylinder, minimizing heat losses, and resulting in higher reaction rates and more heat deposition in the gas



# Closing remarks (3/4)

- ✓ Imposing significantly faster rotational speeds could continue to yield a decreasing trend due to the changes induced in the flow field and resulting thicker thermal boundary layers but it is unlikely that for stoichiometric hydrogen-air mixtures the thresholds will fall below 930 K
- ✓ Hydrocarbons with strong negative temperature coefficient (NTC) regions (faster ignition delay time at lower temperatures) could exhibit a stronger dependence



# Closing remarks (4/4)

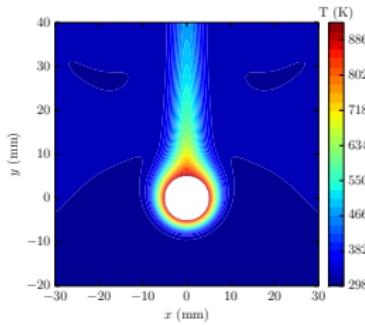
- ✓ Results highlight the importance of capturing properly the interaction of the hot surface with the buoyancy flow induced by the heating of the gas and imposed boundary conditions (rotation) if quantitative numerical predictions of ignition thresholds are sought
- ✓ Hot surface ignition thresholds are not a definite number or a mixture property but vary significantly depending upon a variety of factors such as the state of the hot surface with respect to the combustible gas (i.e. moving or stationary), mode of heat transfer (i.e. forced vs. natural convection), surface material properties, orientation, and **rotation**

# Sponsors

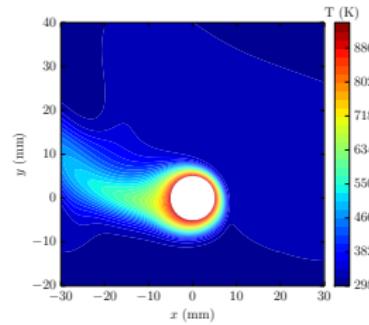


**XSEDE**

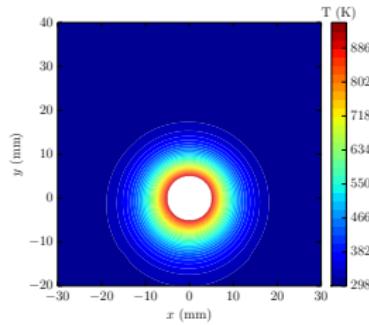
Extreme Science and Engineering  
Discovery Environment



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$$\omega = 240 \text{ rad/s}$$



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