Boundary Layer Ignition Modeling

Stephanie A. Coronel[a,b], Simon Lapointe[a,c], and Joseph E. Shepherd[a]

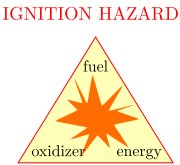
[a]California Institute of Technology, Pasadena, CA 91125
[b]Sandia National Laboratories, Albuquerque, NM 87185
[c] Lawrence Livermore National Laboratory, Livermore, CA 94550

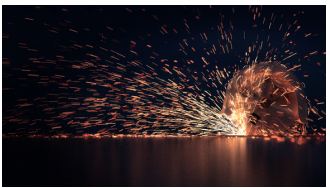
11th U.S. National Combustion Meeting
March 24 – 27, 2019

Motivation

Hot surfaces

- Manufacturing
- Mining
- Aviation
- Nuclear





Additional context

- Hot reactive gas adjacent to cold walls: relevant to HCCI engines that operate at low temperature

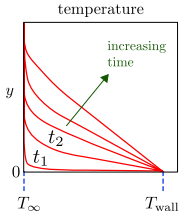
[0]Grinding animation: How to Make Sparks. Blender Guru. November 28, 2012. `https://www.blenderguru.com/tutorials/how-to-make-sparks`

Objective

- Investigate wall normal fluid behavior adjacent to hot wall (species and ignition)
- Use hydrocarbon fuel to simulate engine relevant fuels

Problem setup

- Variation of the classical Rayleigh problem (impulsive heating rather than impulsive acceleration)



Methodology Cont'd

Solution

- Low Mach number reactive Navier-Stokes equations in 1D solved with NGA[1]
- Constant non-unity Lewis number
- Fluid parcel tracking based on "Lagrangian" tracking
- Detailed *n*-hexane mechanism[2] (62 species, 226 rxns)

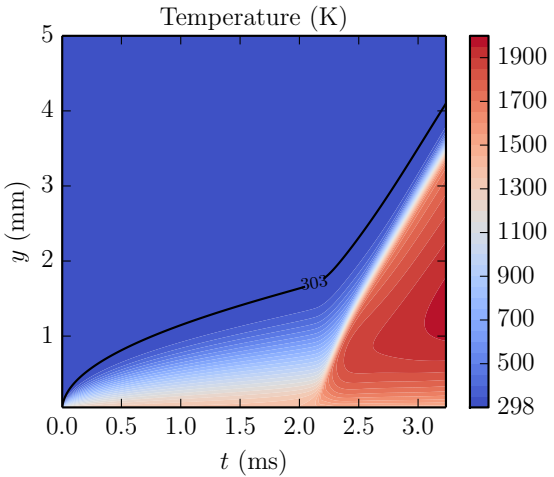
Initial conditions

- $T_0 = 300$ K, $P_0 = 100$ kPa, $\Phi = 0.9$
- $T_{\text{wall}} = 1150$ and 1400 K

[1] O. Desjardins et al., *High order conservative finite difference scheme for variable density low Mach number turbulent flows*, Journal of Computational Physics 227 (2008) 7125-7159.

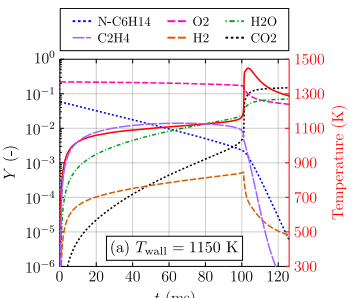
[2] R. Mével et al., *Low temperature oxidation of n-hexane in a flow reactor*, Fuel 126 (2014) 282-293.

Temperature Field: $T_{\text{wall}} = 1400$ K

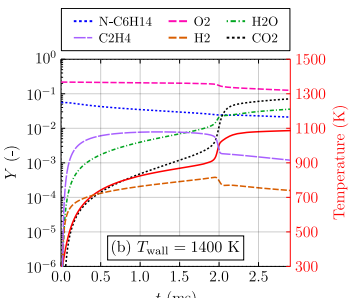


Species History

- Selected fluid parcels originating 0.150 mm from the wall
- Fuel depletion mainly through decomposition of *n*-hexane into smaller fuel molecules



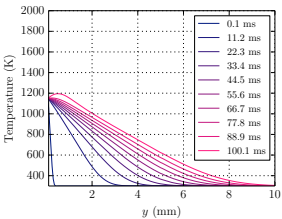
$T_{\text{wall}} = 1150$ K

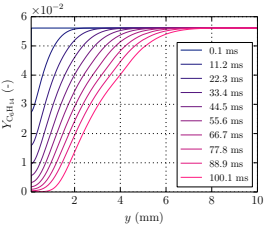


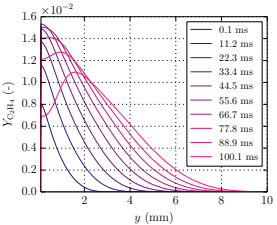
$T_{\text{wall}} = 1400$ K

Temperature and Species Profiles ($t \leq t_{\text{ign}}$)

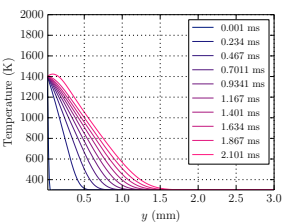
$T_{\text{wall}} = 1150$ K

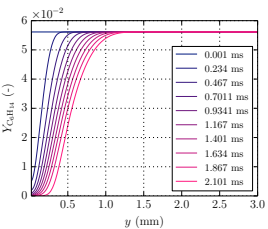


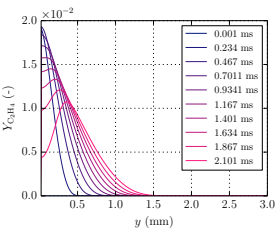




$T_{\text{wall}} = 1400$ K



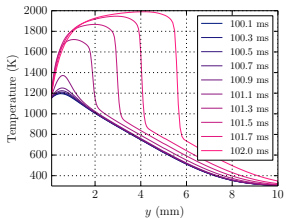


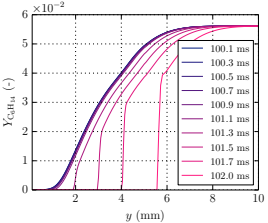


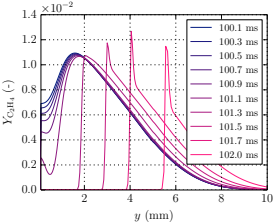
Temperature | *n*-hexane | ethylene

Temperature and Species Profiles ($t > t_{\text{ign}}$)

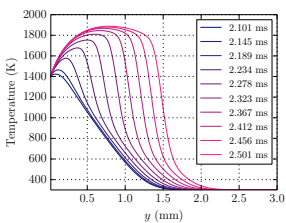
$T_{\text{wall}} = 1150$ K

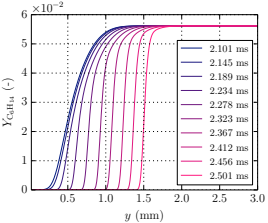


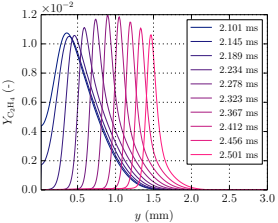




$T_{\text{wall}} = 1400$ K



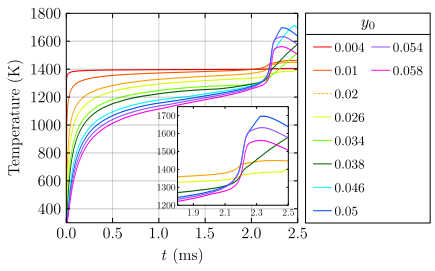


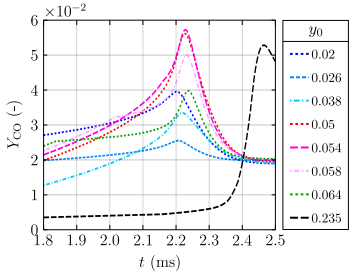


Temperature | *n*-hexane | ethylene

Ignition Location: $T_{\text{wall}} = 1400$ K

- Temporal evolution of igniting fluid parcel (y_0 units in mm)
- Temperature criterion not possible
- Temperature jumps range from $100 - 400$ K





- Species mass fraction evolution
- CO has a distinct peak at ignition

Conclusions

- Significant decomposition of *n*-hexane prior to ignition
- Mainly igniting fuel is ethylene within thin region in thermal boundary layer
- The width of depleted regions are $7 - 10\%$ thermal boundary layer thicknesses
- Ignition always occurs some distance away from the wall
- The use of fluid parcel tracking allowed us to analyze the behavior of several fluid parcels close to the hot wall
- The temperature and species mass fraction of CO allowed us to pinpoint the igniting fluid parcel based on the ignition criterion that uses the peak in CO to mark ignition