103-species n-dodecane Skeletal Mechanism

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ECN Modeling Web meeting
November 15th 2011

Mechanism Reduction Methodology

~ 20 times reduction

Detailed Mechanism (from LLNL)
2115 species, 8157 reactions

DRG – X*

369 species,1495 reactions

DRGASA

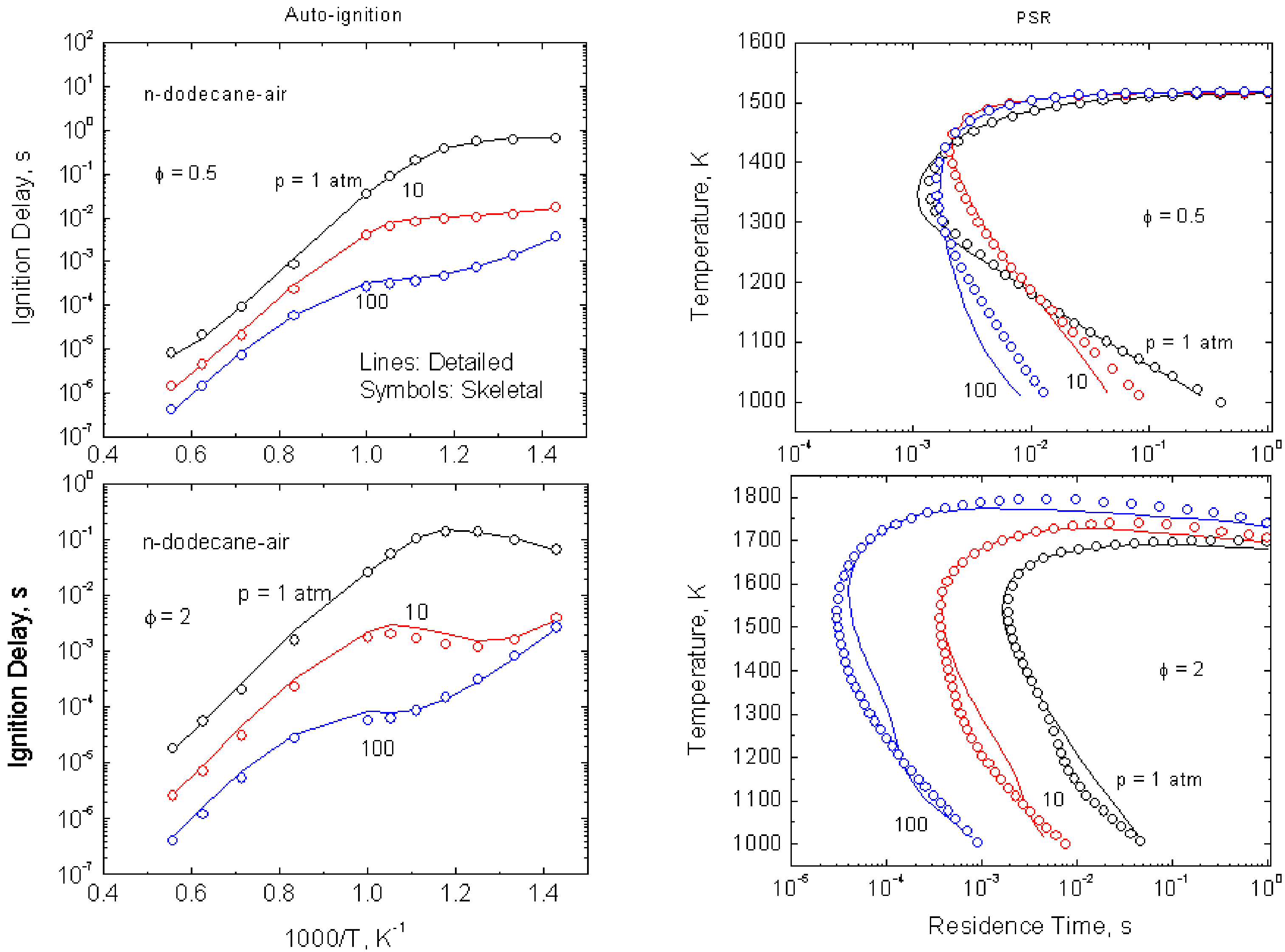
Skeletal Mechanism*:
103 species,
370 reactions

Range of operation:
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

***Three Dimensional Simulations of Diesel Sprays using n-dodecane as a Surrogate (B-04): Fall Technical Meeting of the Eastern States Section of the Combustion Institute, University of Connecticut, CT, USA. Oct 9-12, 2011**

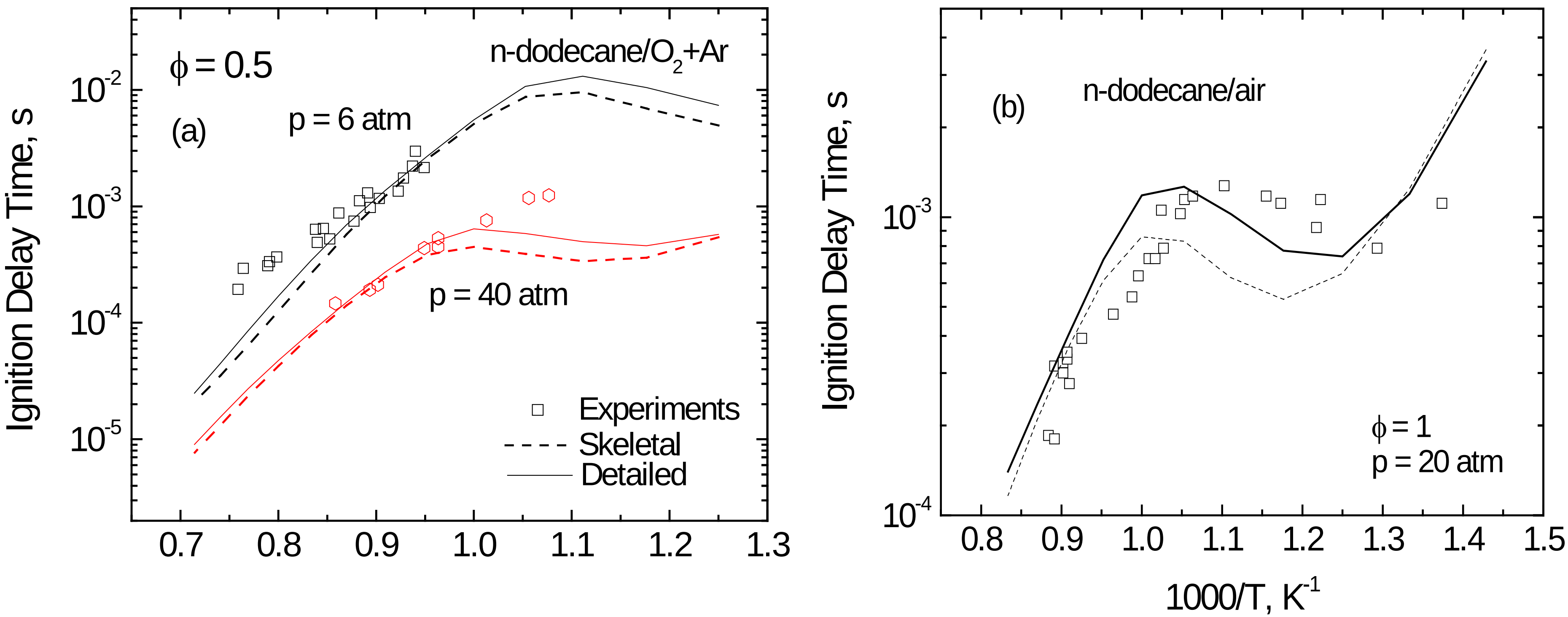
*** T. Lu, M. Plomer, Z. Luo, S.M. Sarathy, W.J. Pitz, S. Som, D.E. Longman, 1A03. *US National Combustion Institute meeting, 2011***

Detailed vs. Skeletal mechanism



Comparison of the 103-species skeletal mechanism with the detailed mechanism for ignition delays and extinction temperature profiles in PSR

Ignition Delay Validation

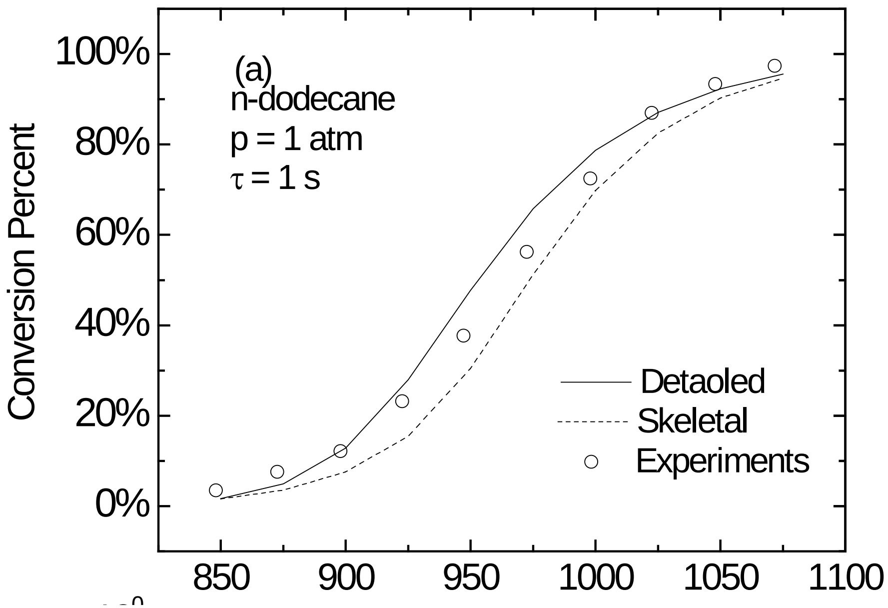


Black symbols: experimental data from: Davidson et al. Combustion and Flame 2008

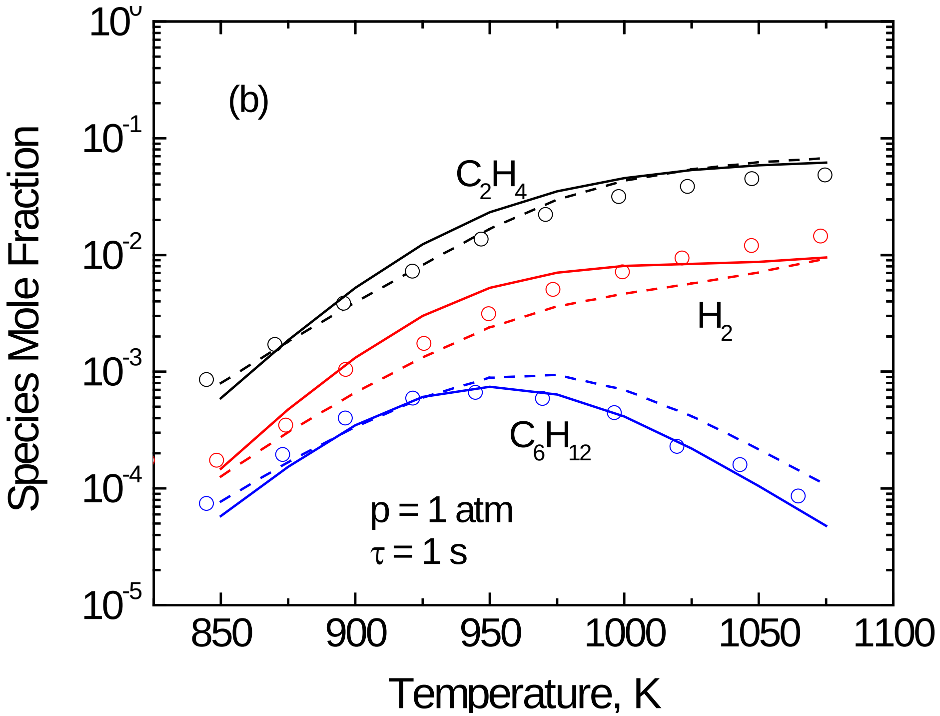
Experimental data from: Vasu et al. Proc. of Combustion Institute 2009

Red symbols: experimental data from: Shen et al. Energy and Fuels 2009

Validation against Jet Stirred Reactor Data



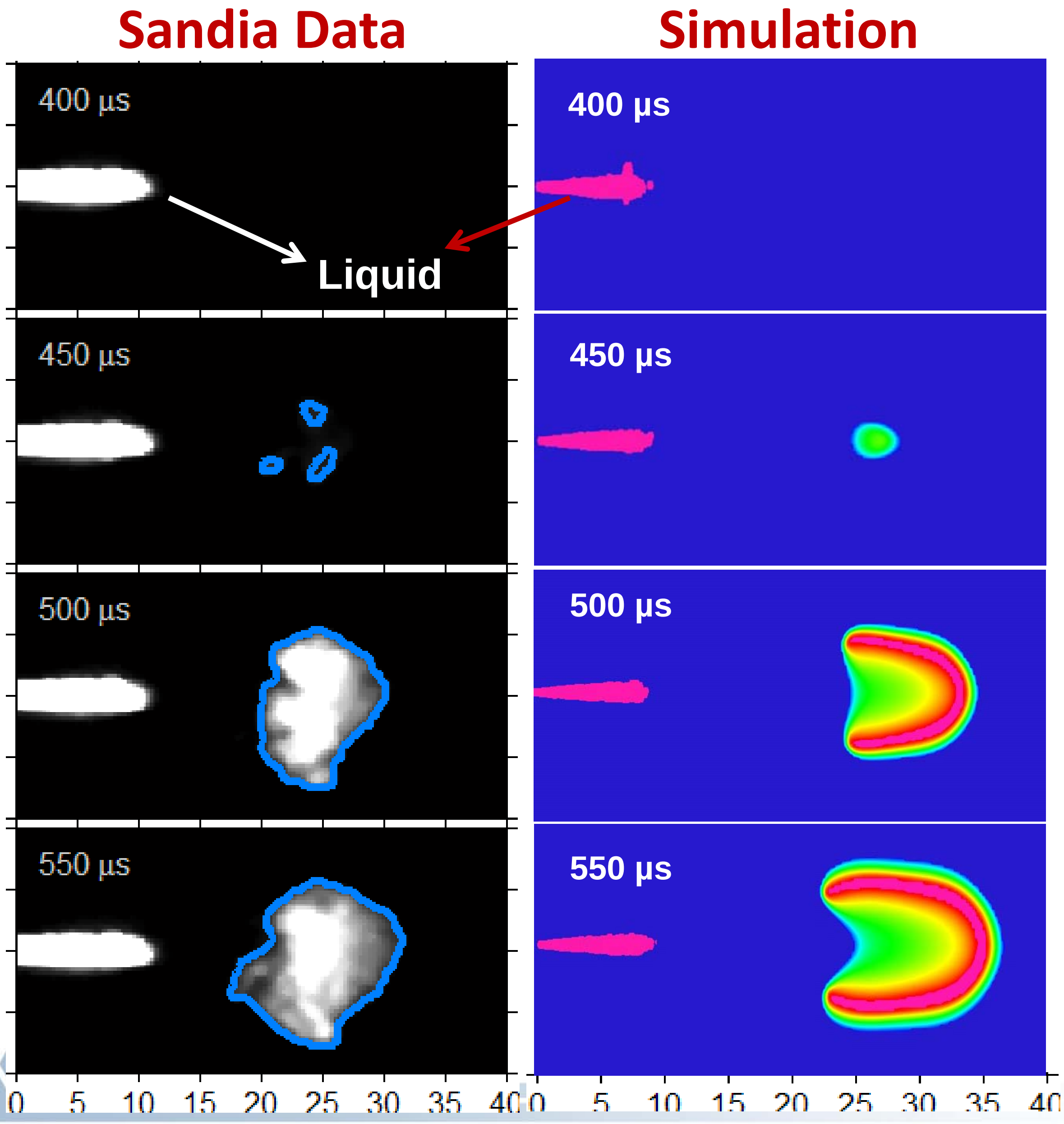
Comparison of calculated and measured conversion percent of n-dodecane thermal decomposition in JSR, at p =1 atm and τ=1s



Comparison of calculated and measured species profiles in JSR, at p = 1 atm and τ = 1s

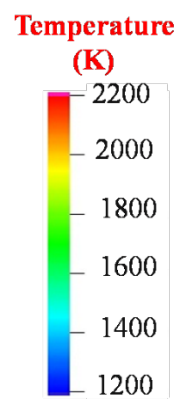
Experimental data from: Herbinet et al. *J. Anal. Appl. Pyrolysis* 2007

Liquid Length and Ignition Location

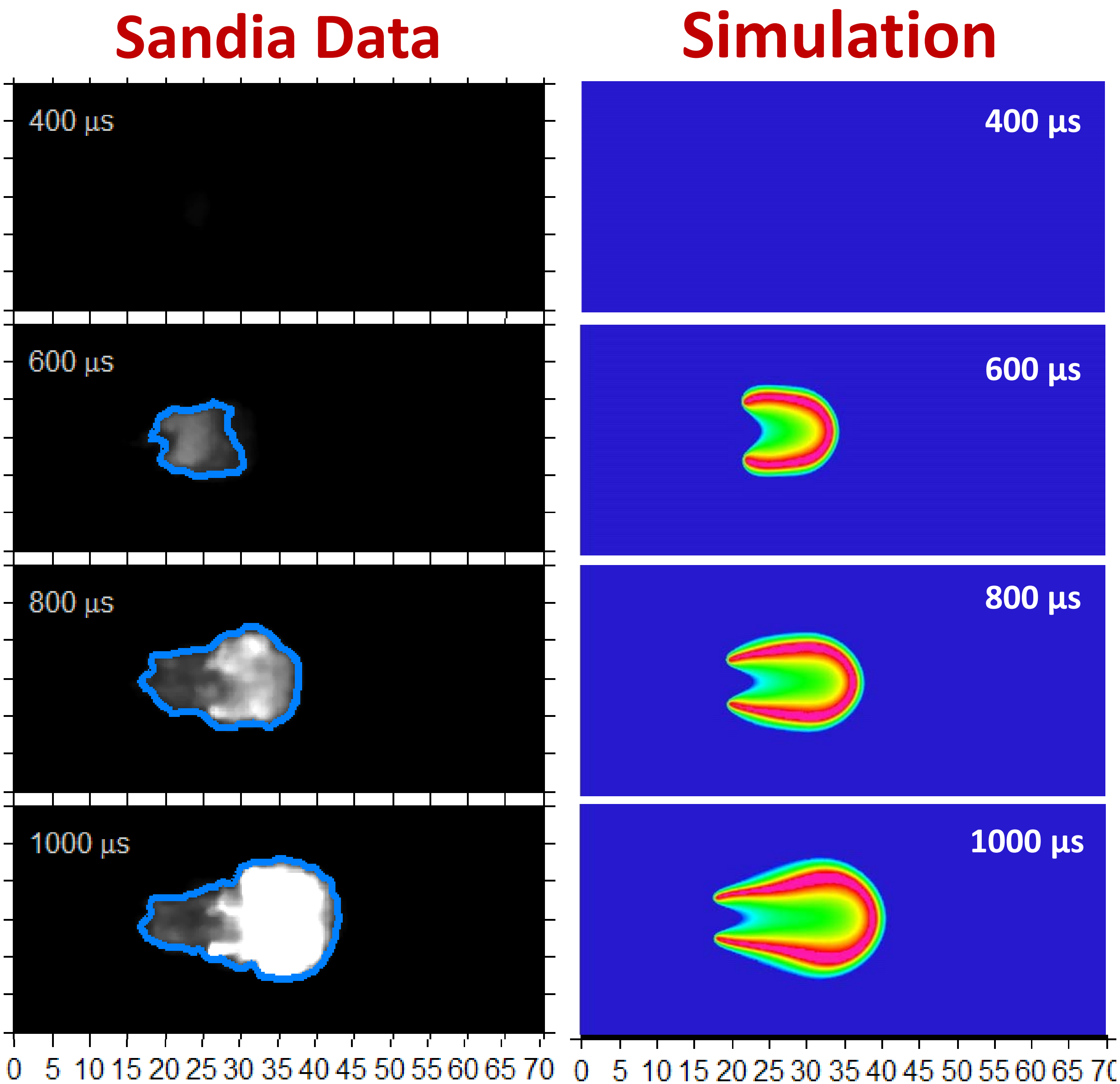


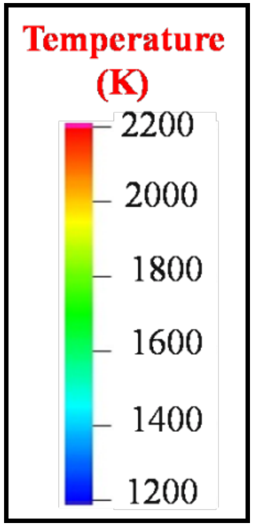
Experiments:
Natural Luminosity high-speed imaging for detection of ignition delay

Simulation:
Temperature contours plotted to capture ignition location and delay



Flame Development at 900K

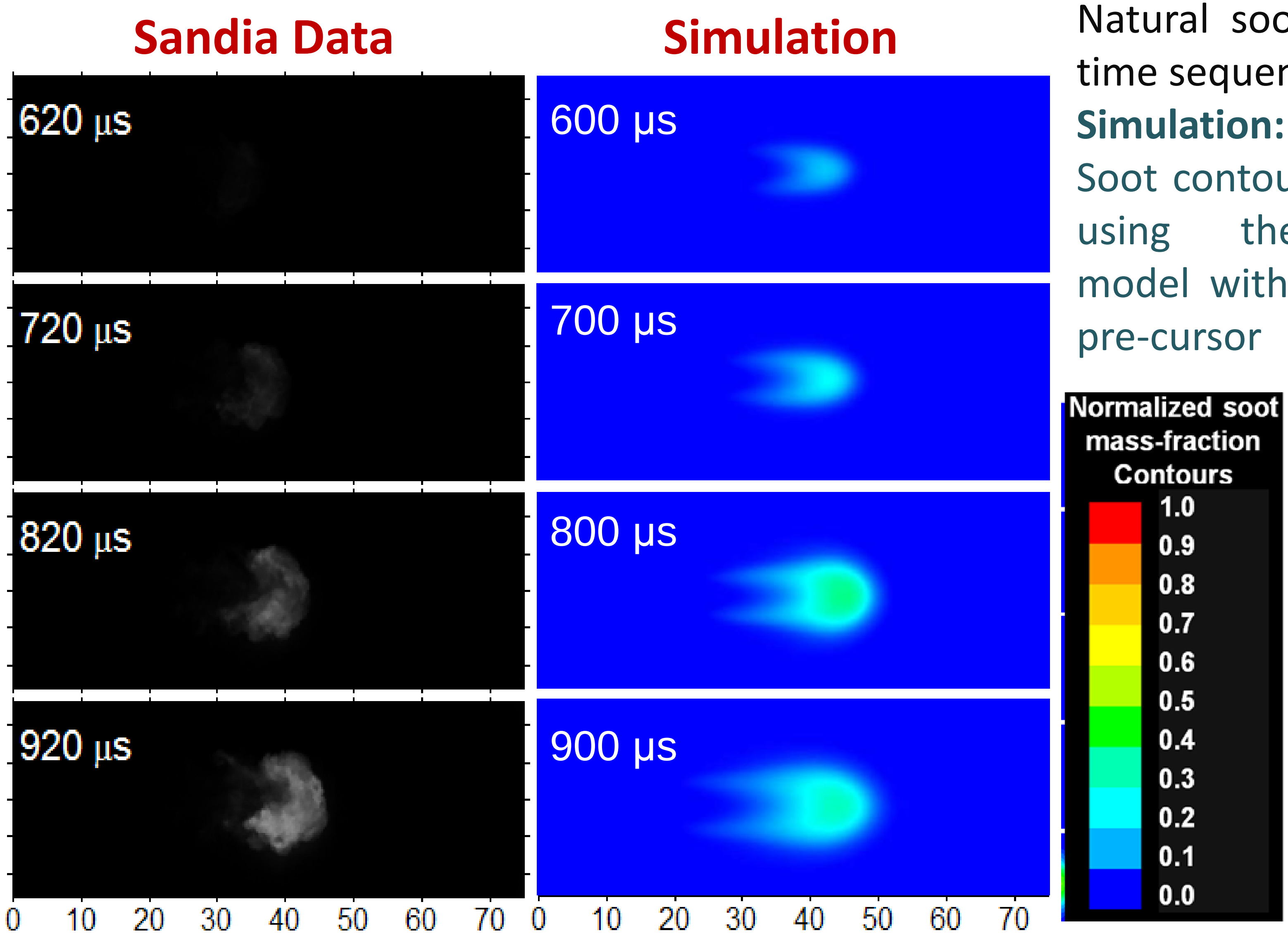




Experiments:
Natural Luminosity high-speed imaging for detection of ignition delay

Simulation:
Temperature contours plotted to capture flame development

Soot Distribution @ 900K

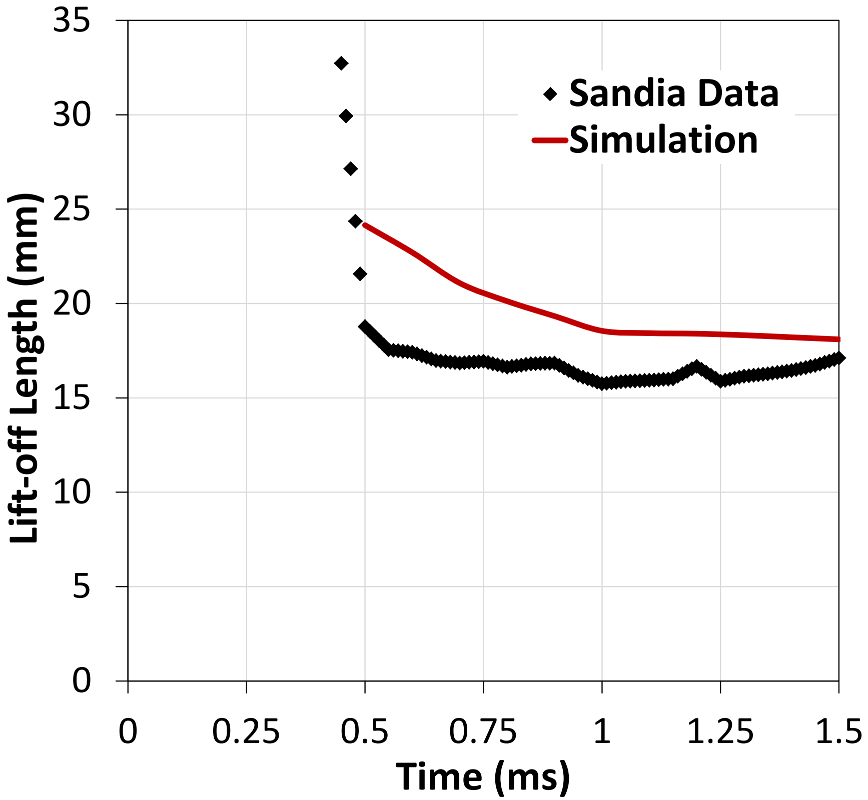


Experiments:
Natural soot Luminosity time sequence at IFP

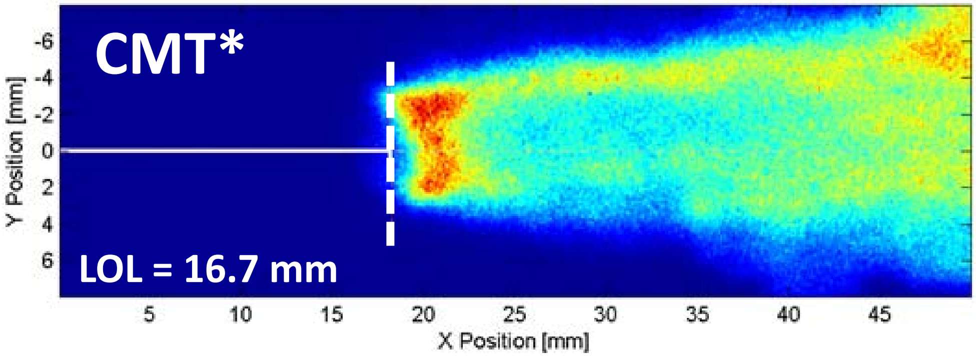
Simulation:
Soot contours calculated using the Hiroyasu model with C_2H_2 as the pre-cursor

Ignition Delay and Flame lift-off Length

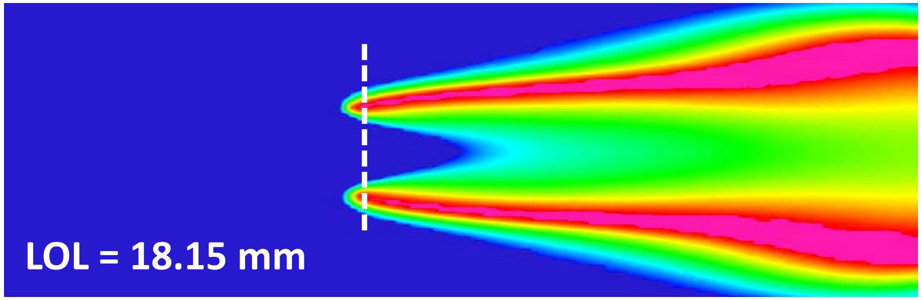
@ 900 K	Ignition Delay (ms)	Lift-off Length (mm)
Sandia Data	0.440	16.50
Simulation	0.500	18.15



OH chemiluminescence

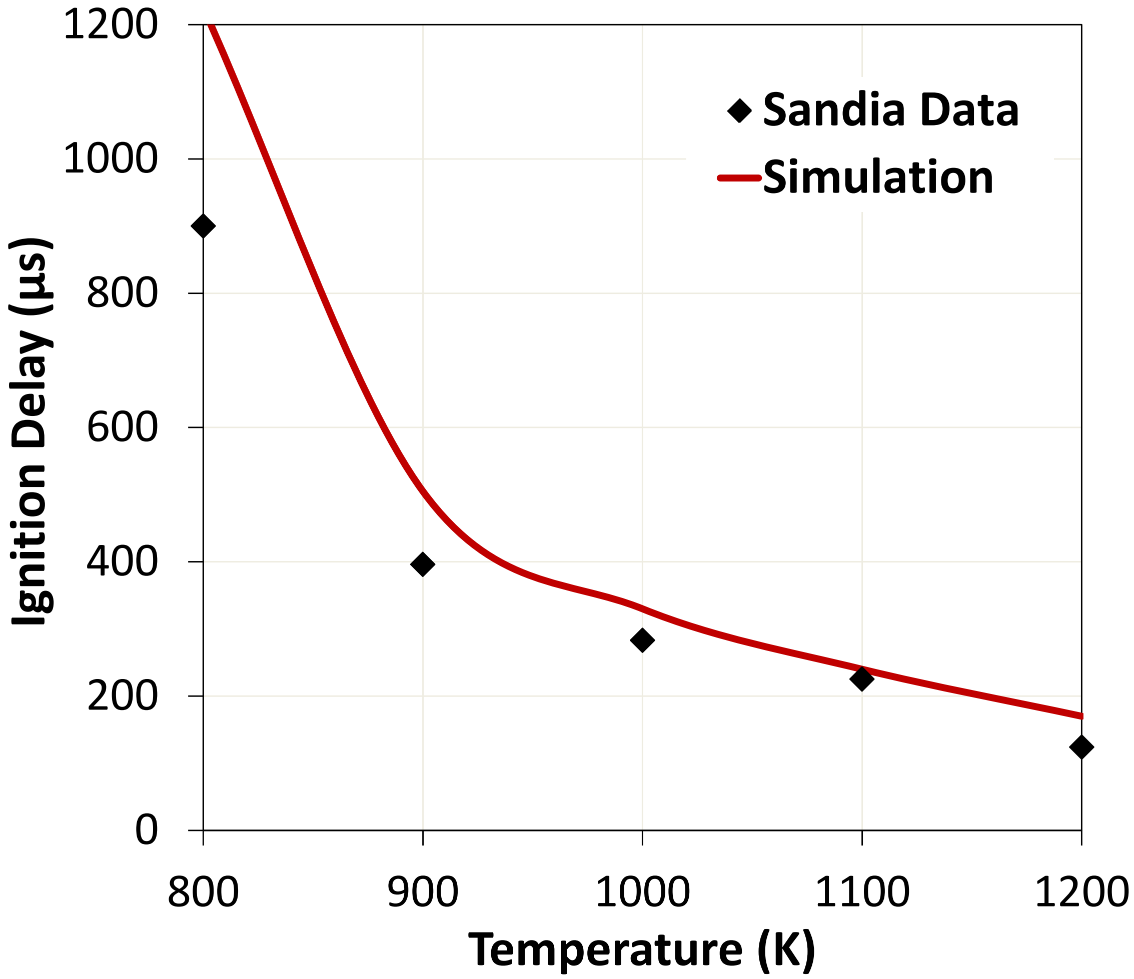


Simulation



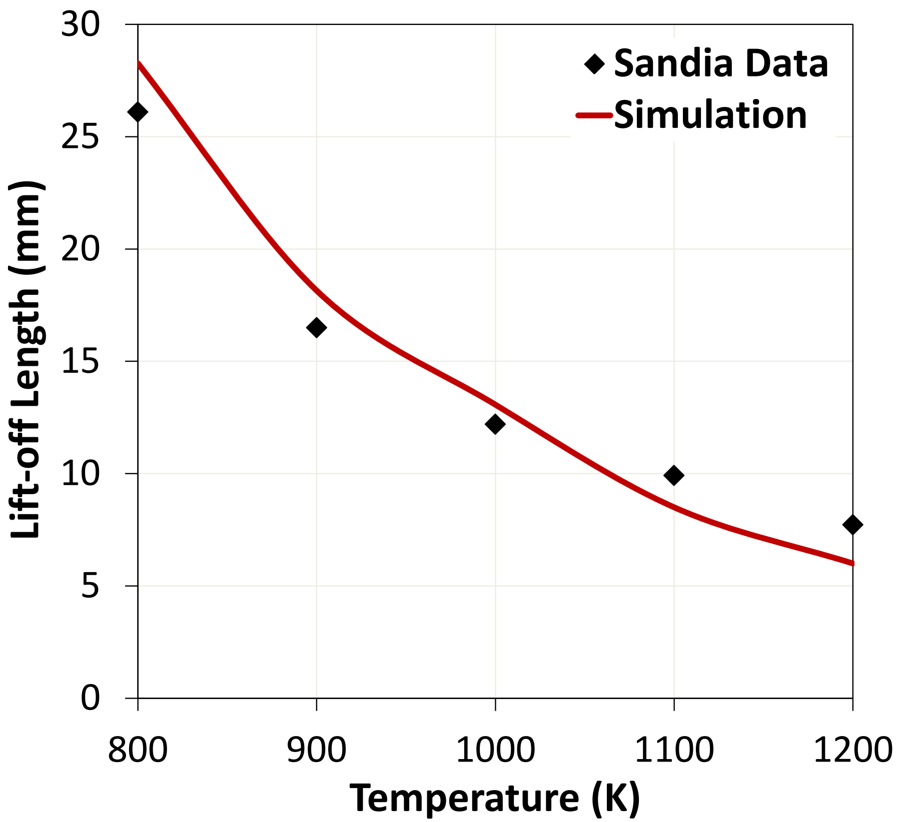
*http://www.cmt.upv.es/ECN07.aspx

Effect of Ambient Temperature



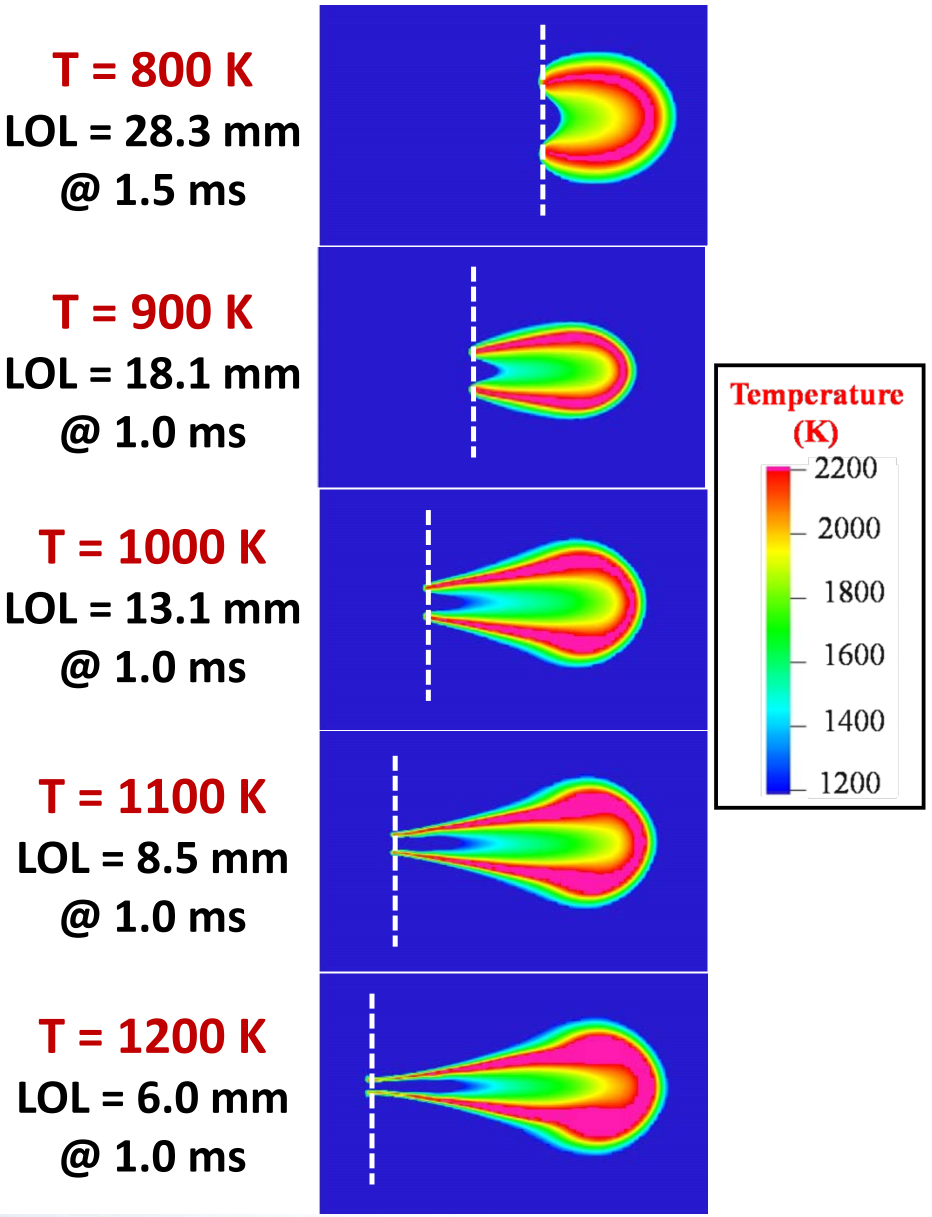
- Ignition delay decreases with increase in ambient temperature
- In general, ignition characteristics are well predicted by the mechanism
- At lower ambient temperatures ignition delay is over predicted

Effect of Ambient Temperature



In general, flame lift-off characteristics are well captured by the mechanism, especially in the medium temperature range!

Simulations

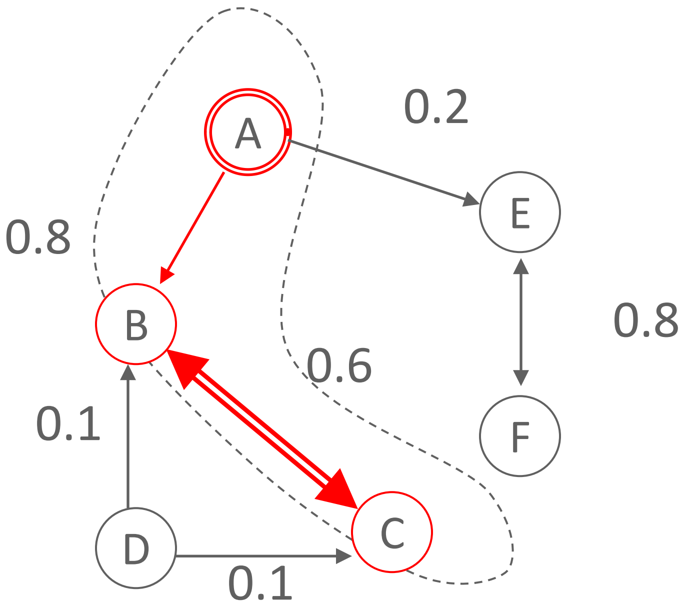


Backup

DRG vs. DRG-X*

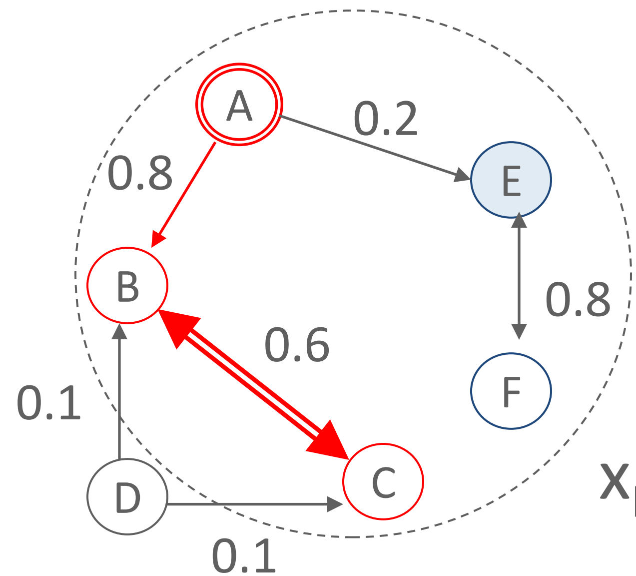
DRG

- ✓ Error tolerance for each species fixed during the reduction process.



DRG-X

- ✓ Species-specific error tolerance based on expert knowledge
- ✓ Reactions with low uncertainty → species with low error tolerance
- ✓ Species of interest can be assigned low error tolerance also
- ✓ Error tolerance for HRR is also specified



$X_E < 0.1$

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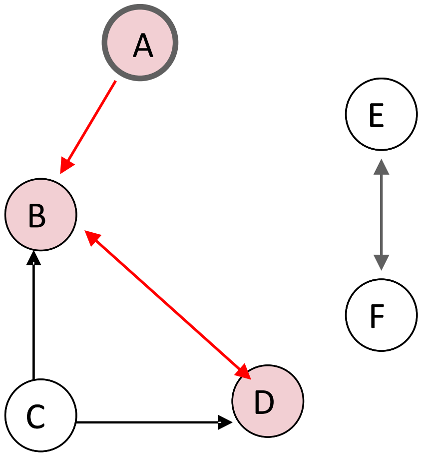
Step1: Skeletal Reduction with Directed Relation Graph (DRG)

- **DRG**(*Lu &Law, 2005;Luo et al, 2010*): a graph-based algorithm to eliminate unimportant species
  - Mapping species relation to a graph:

$$r_{AB} \equiv \frac{\max_i \left(\left| \nu_{A,i} \omega_i \delta_{Bi} \right| \right)}{\max_i \left(\left| \nu_{A,i} \omega_i \right| \right)} \qquad \delta_{Bi} = \begin{cases} 1, & \text{If reaction i involves species B} \\ 0, & \text{otherwise} \end{cases}$$



  - A→B: (if $r_{AB} > \varepsilon$; ε: threshold error)

  if A is kept in skeletal mechanism, B should also be kept

- Advantages of DRG:
  - High efficiency(Linear time reduction)
  - Fully automated