Effects of Aromatic Fuel Blending on the Extinction Limits and Soot Formation of n-Decane Diffusion Flames

Sang Hee Won, Wenting Sun, Xiaolong Gou and Yiguang Ju

Mechanical and Aerospace Engineering
Princeton University

Introduction: Surrogate Fuel Model Development

- **Jet Fuel includes various hydrocarbon molecules:**
  - normal, branched, and cyclo alkanes, and aromatics
- **MURI team selected surrogate jet fuel components**
  - n-decane, methyl-cyclohexane, n-propyl- and trimethyl-benzenes, toluene…

By matching H/C ratio, sooting index, burning rates, ignition time…

- **Example: Gasoline Surrogate model (PRF+1)**
  - Blending of toluene to n-heptane and iso-octane to meet both burning and soot formation targets
- **Challenge 1**: How does the kinetic coupling between aromatics and normal alkanes affect burning rate, extinction limit, and soot formation?
- **Challenge 2**: How to generate an efficient kinetic reduction method for direct numerical simulation?

Objectives

- Investigate the kinetic and transport coupling effects of toluene and trimethyl benzene blending in n-decane on extinction limits and heat release rate using counterflow diffusion flames
- Measure the effects of toluene blending in n-decane on soot formation, flame temperature, and OH concentration by using laser induced incandescence (LII), Rayleigh scattering, and LIF
- Develop a dynamic multi-scale model for kinetic mechanism reduction

Research Projects in 2008

1. Experimental investigation of aromatics and n-decane kinetic coupling on diffusion flame extinction limits
2. Numerical investigation of n-decane and toluene kinetic coupling on extinction limits
3. Measurements of soot formation of toluene blended n-decane diffusion flames
4. A dynamic multi-scale model and P-MARS

CASE

PENNSTATE

UIC

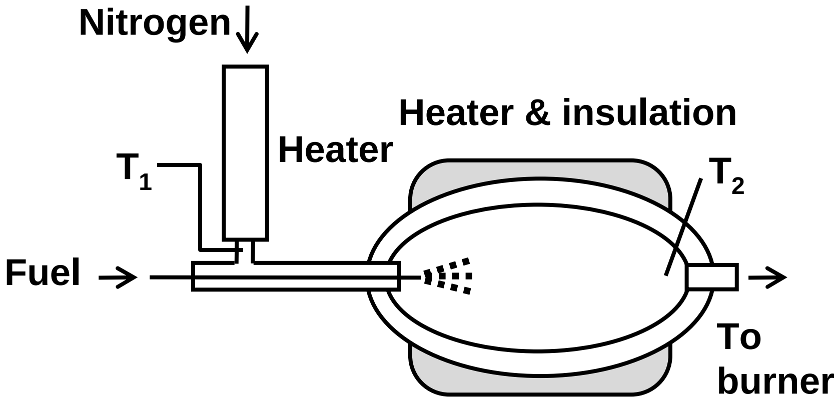
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

UNITED STATES AIR FORCE

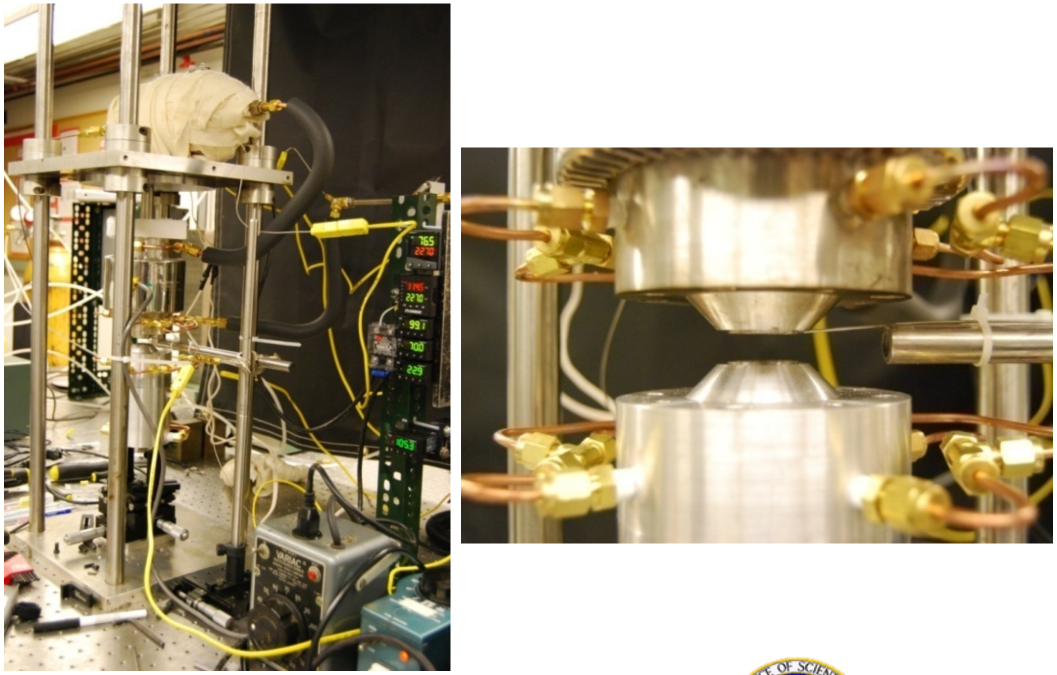
1. Experimental Studies of Diffusion Flame Extinction Limits

(Fuel Vaporization and Counterflow Burner)

- **Integration of liquid fuel evaporation system with counterflow flame burner**
  - Using FTIR measurements to check thermal decomposition and concentration variation: Concentration fluctuation < 1%

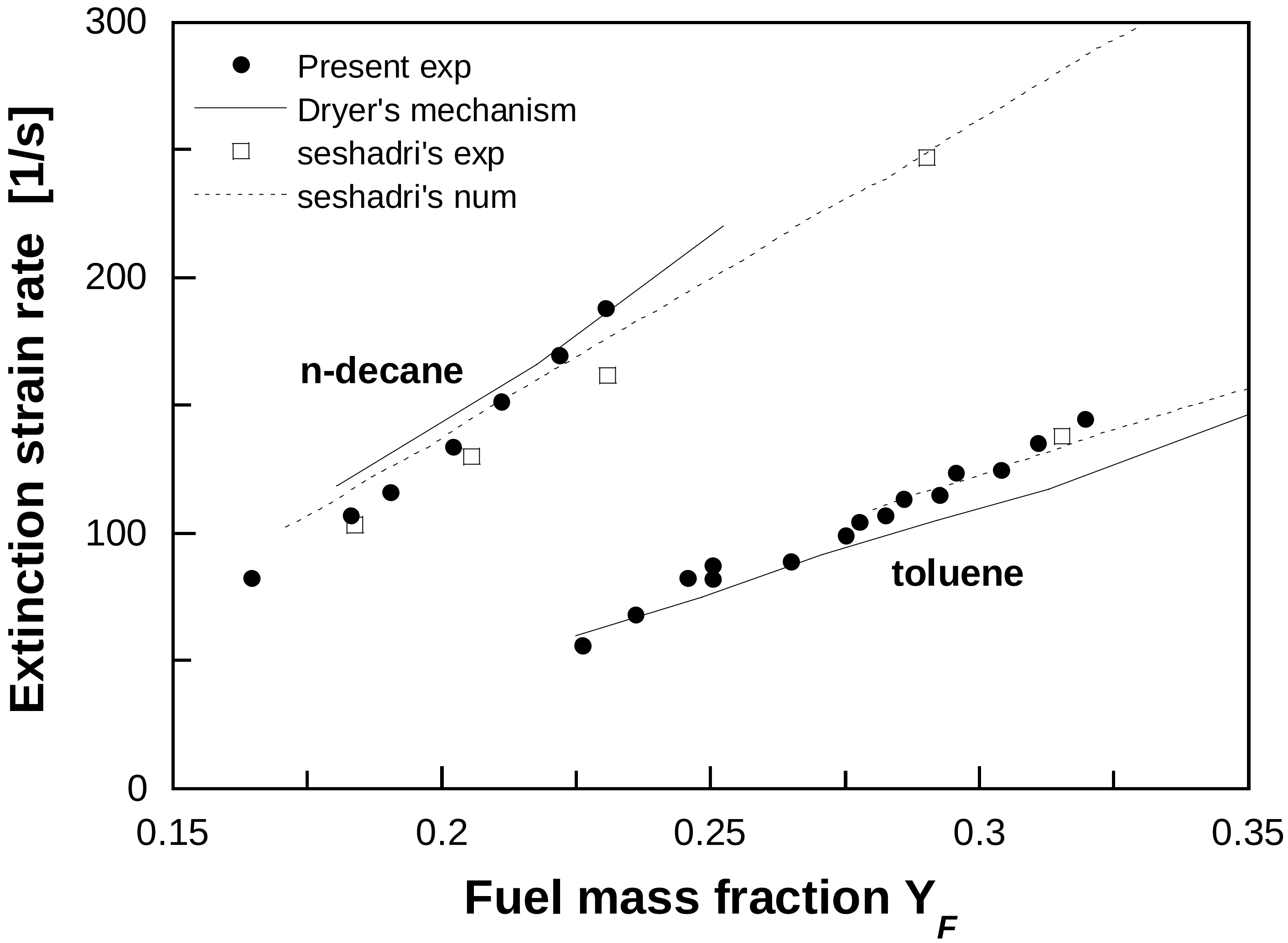


Schematics of evaporation system

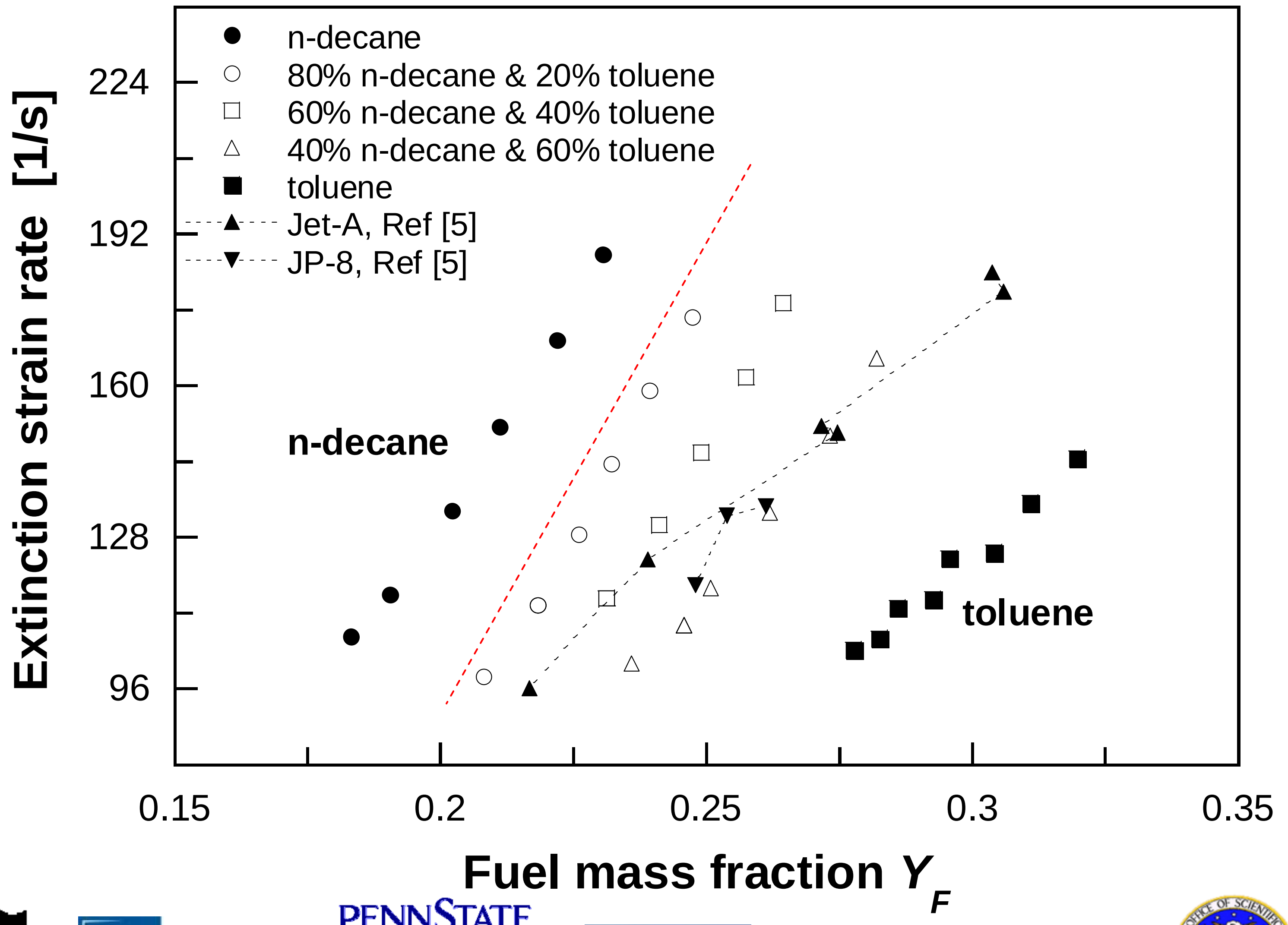


CASE PENNSTATE UIC

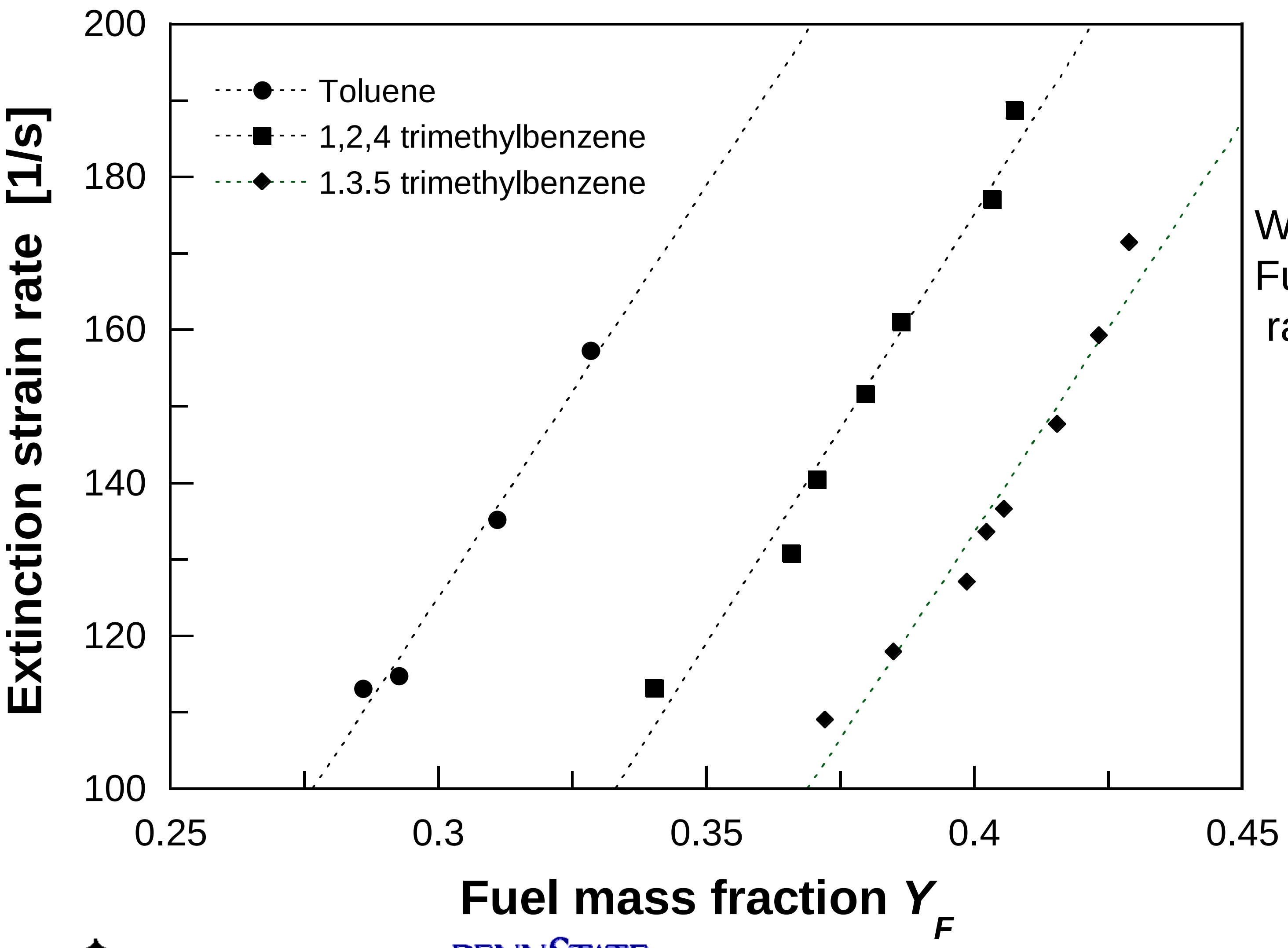
Extinction Strain Rates of Toluene- and n-Decane-Air Diffusion Flames: Validation



Extinction Strain Rates of Toluene Blended n-Decane–Air Mixtures



Extinction Strain Rates of 1,2,4- and 1,3,5-Trimethylbenzene-air Diffusion Flames

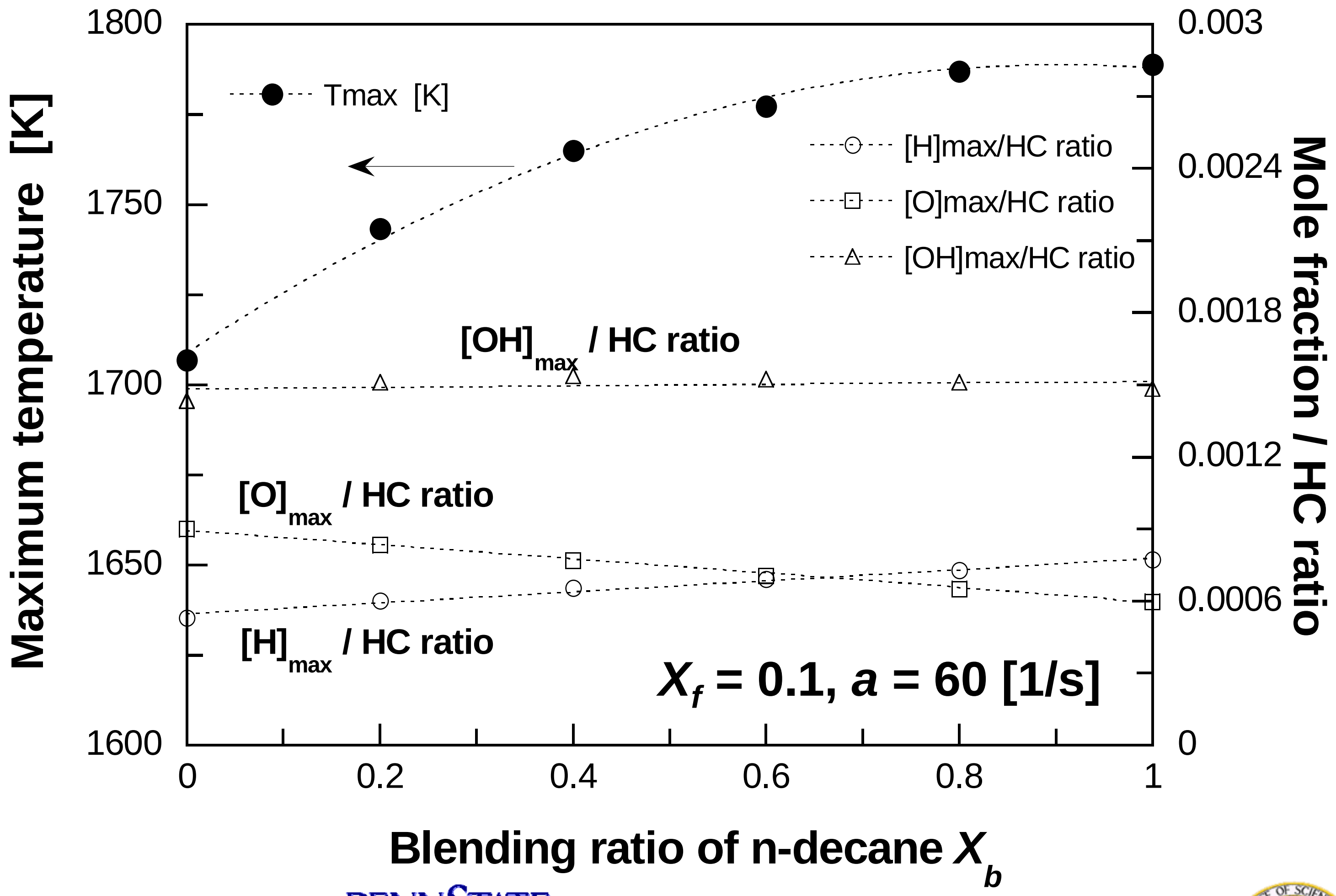


What controls the Fuel oxidation rate?

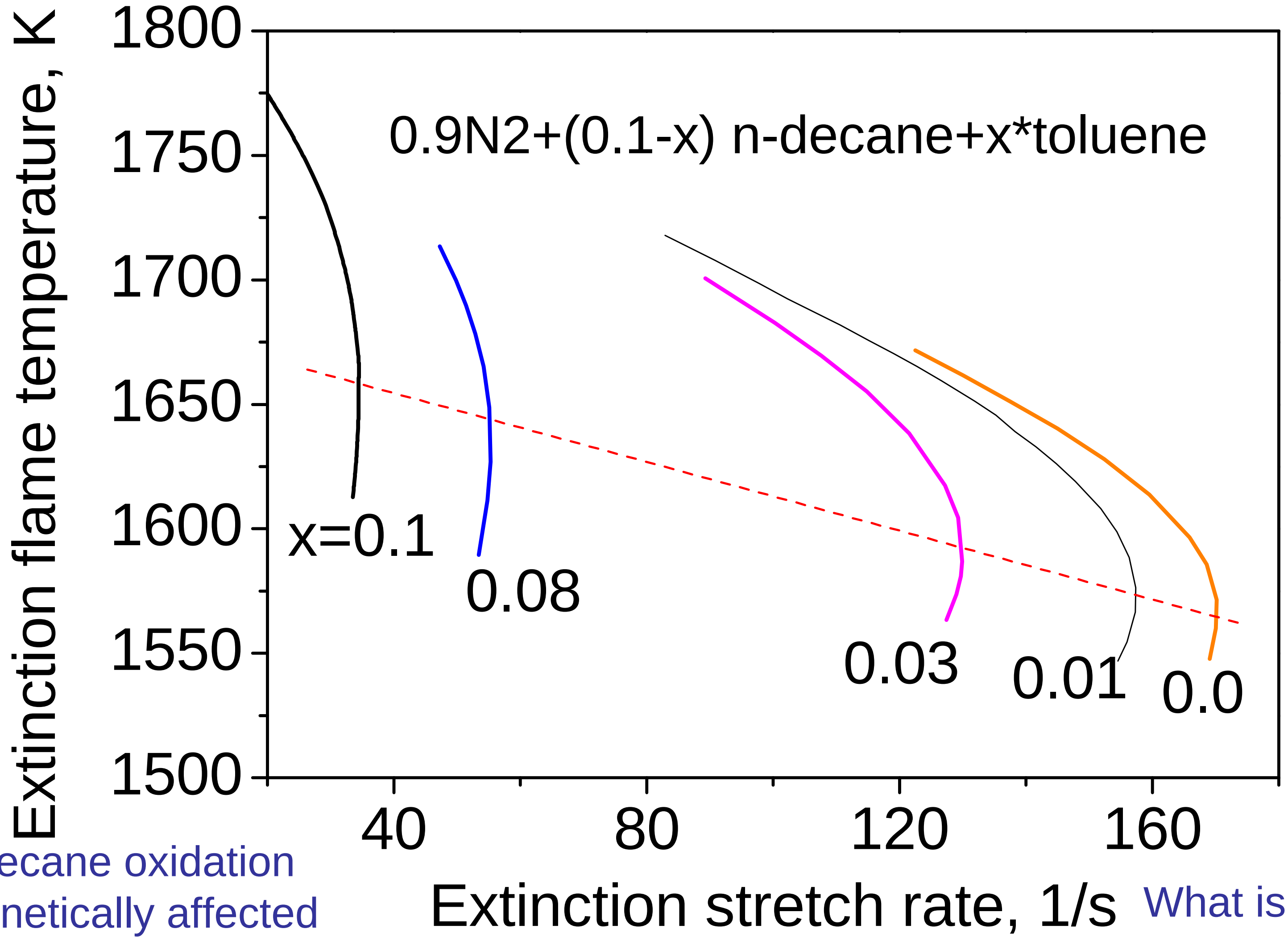
2. Numerical Simulation of n-Decane/Toluene Extinction Limit

(Understanding of kinetic coupling between aromatic/alkane)

How does H/C ratio affect radical pool concentration?



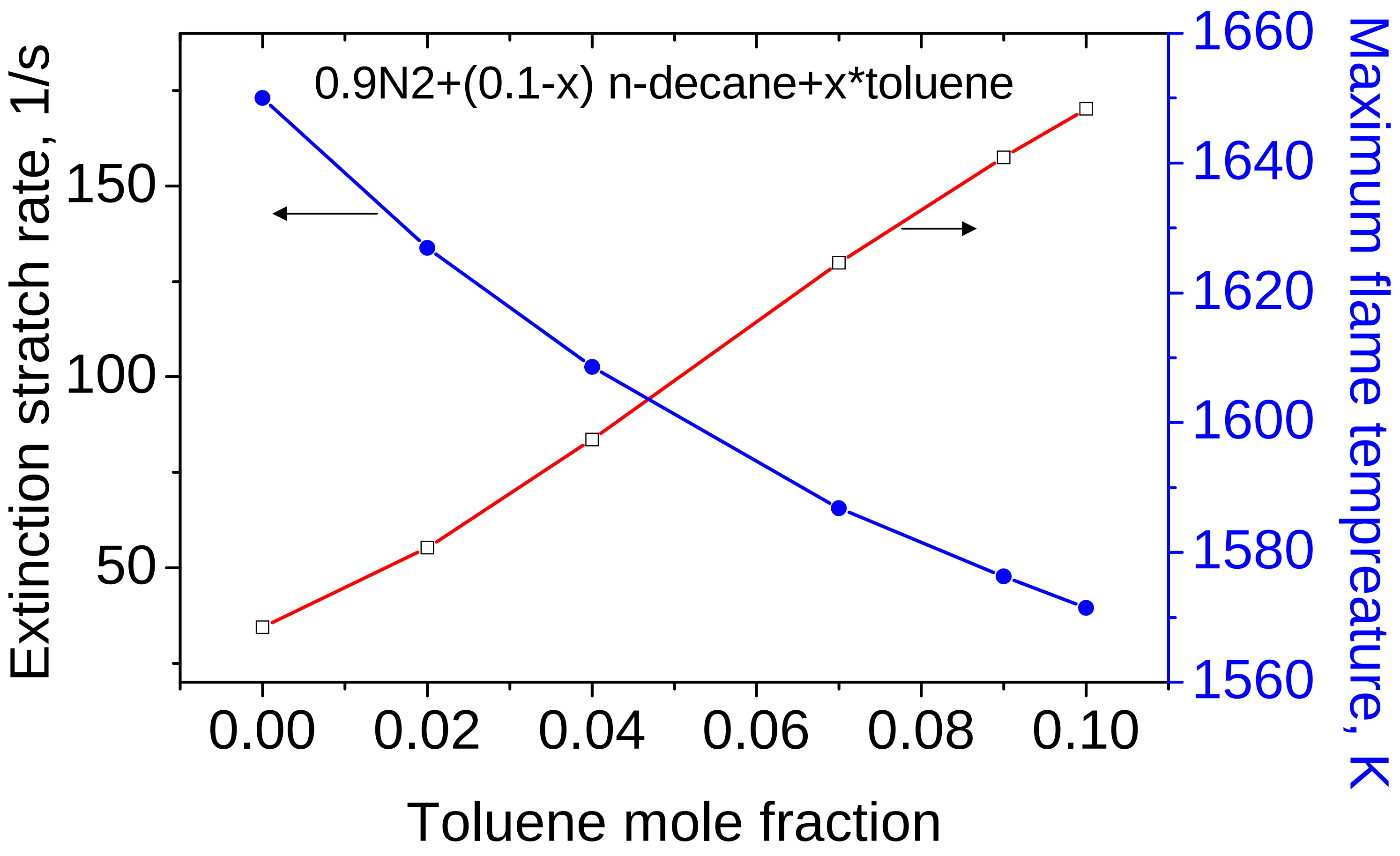
Flame Temperature and Extinction Limit vs. Stretch Rate



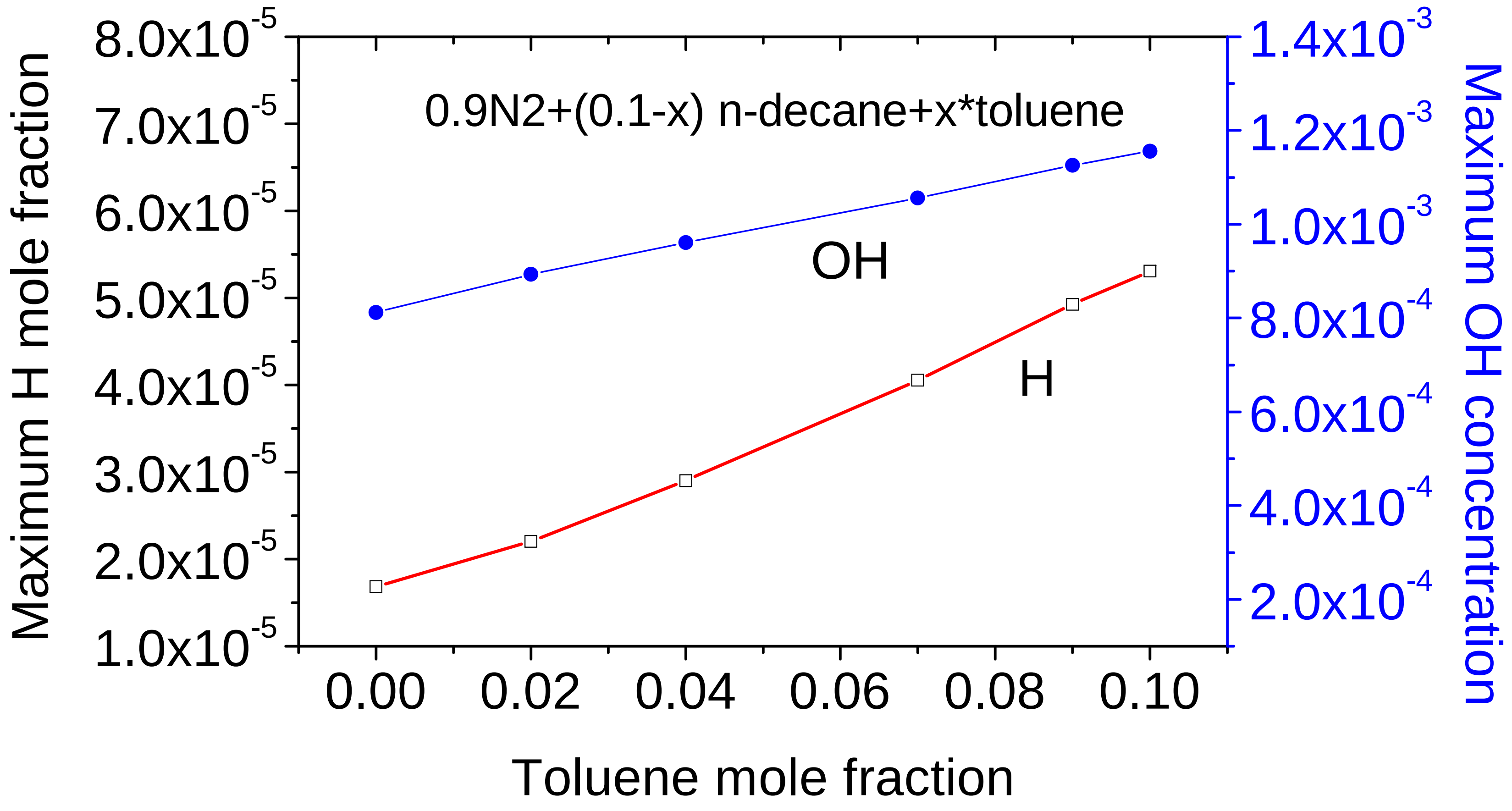
n-Decane oxidation
is kinetically affected
by toluene addition.

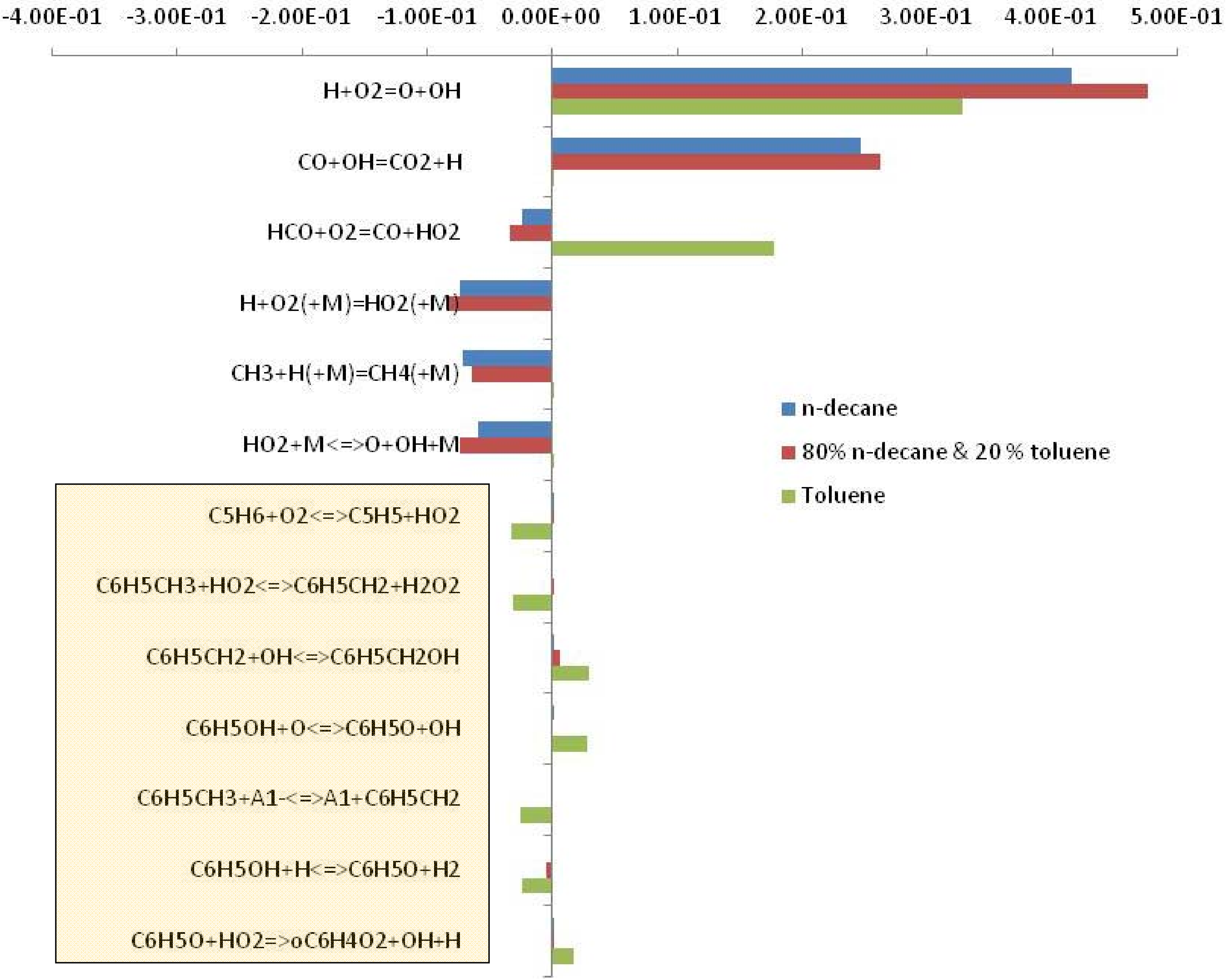
What is the role
of OH concentration?

Extinction Strain rate vs. Toluene Blending Mole Fraction



Maximum OH and H Mole Fractions on Toluene Blending





-4.00E-01
-3.00E-01
-2.00E-01
-1.00E-01
0.00E+00
1.00E-01
2.00E-01
3.00E-01
4.00E-01
5.00E-01
H+O2=O+OH
CO+OH=CO2+H
HCO+O2=CO+HO2
H+O2(+M)=HO2(+M)
CH3+H(+M)=CH4(+M)
HO2+M<=>O+OH+M
C5H6+O2<=>C5H5+HO2
C6H5CH3+HO2<=>C6H5CH2+H2O2
C6H5CH2+OH<=>C6H5CH2OH
C6H5OH+O<=>C6H5O+OH
C6H5CH3+A1-<=>A1+C6H5CH2
C6H5OH+H<=>C6H5O+H2
C6H5O+HO2=>oC6H4O2+OH+H
🟦 n-decane
🟥 80% n-decane & 20 % toluene
🟩 Toluene

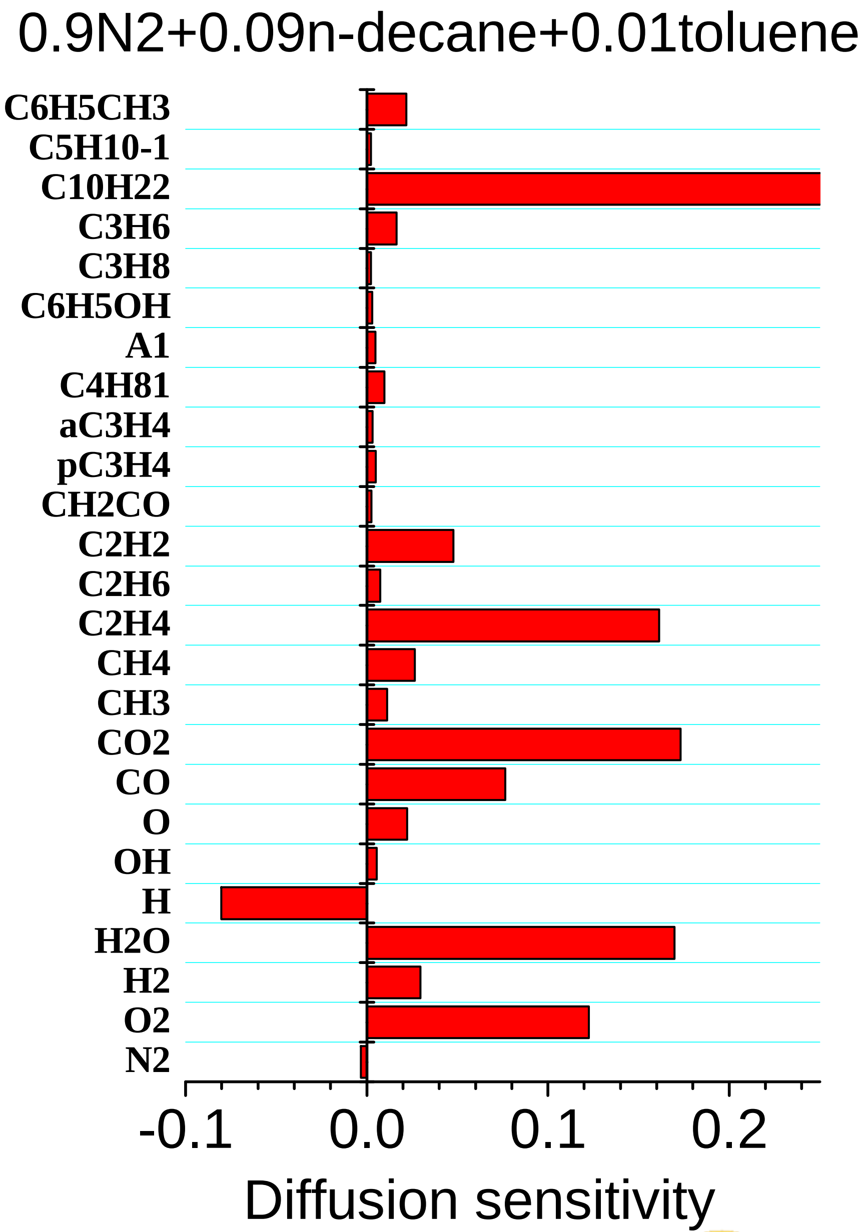
Thermal effect via diffusion:
n-decane, toluene, O_2, CO_2, CO

Jump condition of diffusion flames

$$\rho D_i \frac{dY_F}{dx}\bigg|_{0-}^{0+} = \int_0^{\delta} \omega_i dx$$

Kinetic effect via diffusion:
H, O, OH…

Sensitivity of thermal conductivity



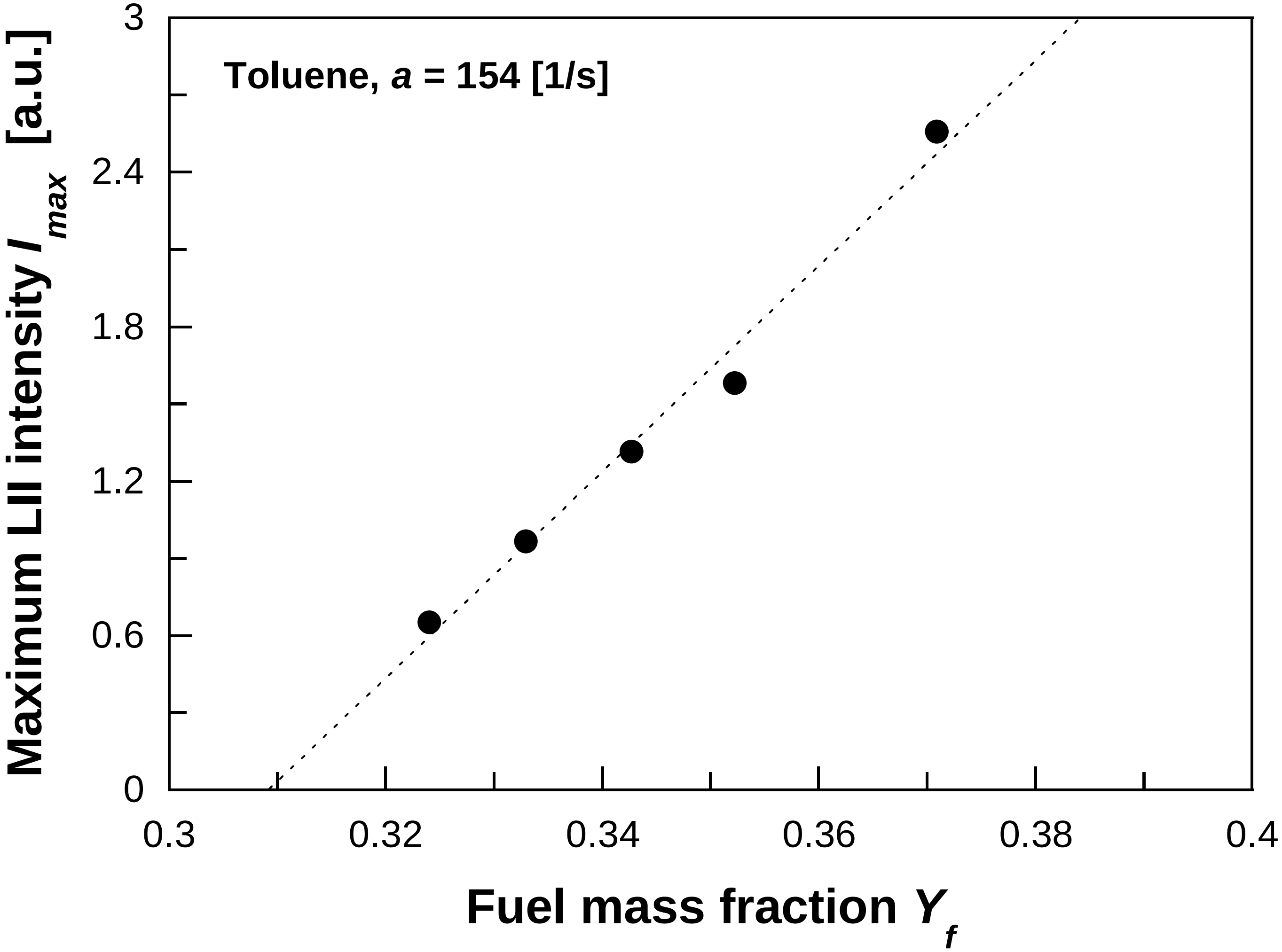
3. Experimental Measurements of Soot Formation & Temperature Using Laser Induced Incandescence & Rayleigh Scattering

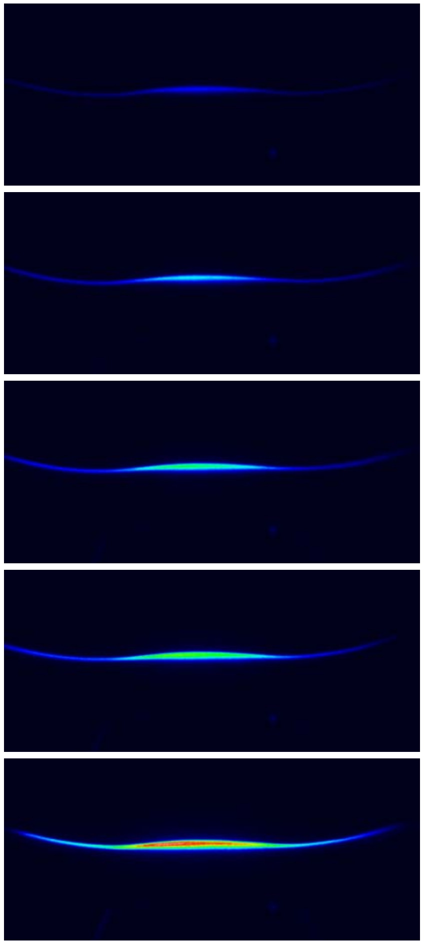
- Nd:YAG Laser : Quanta-Ray (532 nm), Cobra-stretch dye laser
- ICCD Camera : PIMAX-Gen II (Princeton Instrument)
- LII : narrow band pass filter (420 nm)

Photo for Rayleigh scattering and LII

Measured Soot Volume Fraction

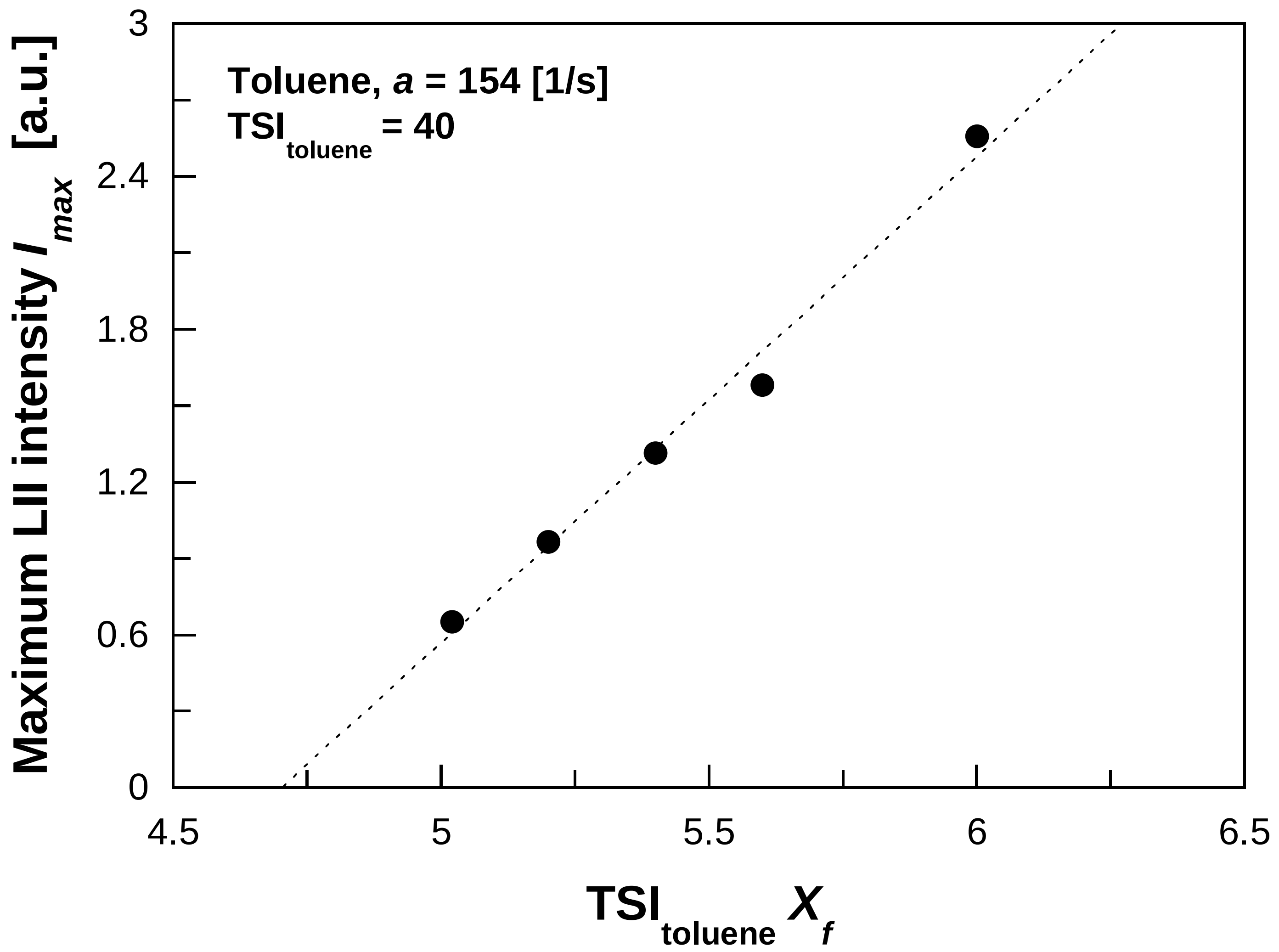
toluene diffusion flame



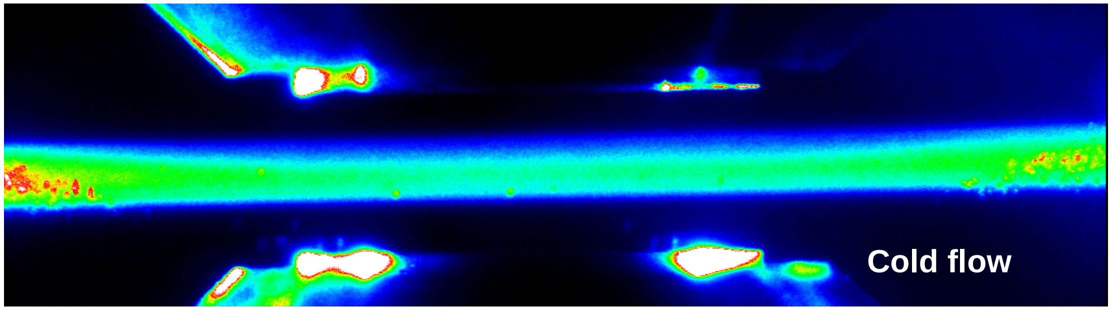


Measured Soot Formation vs. Predicted TSI

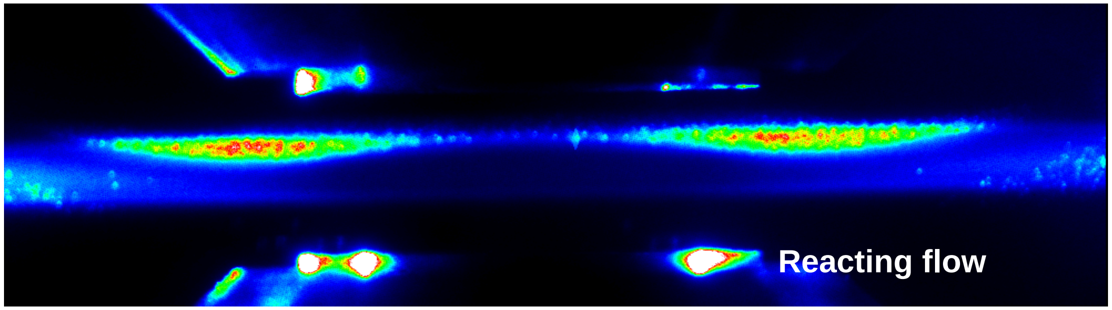
toluene diffusion flame



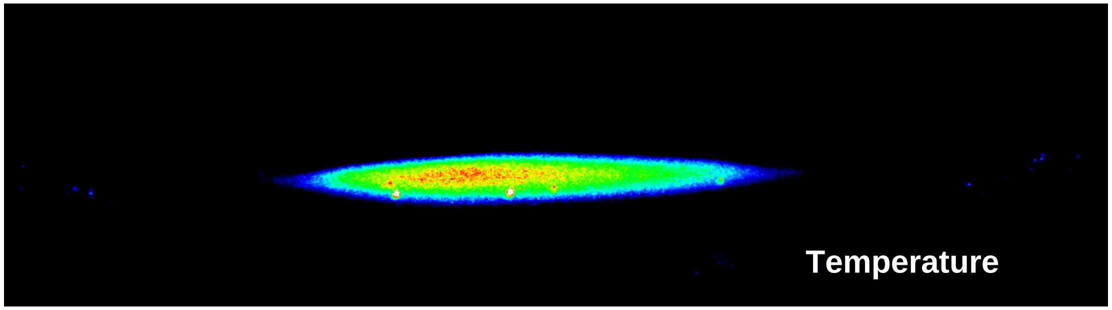
Flame Temperature Measurement using Rayleigh Scattering



Cold flow



Reacting flow



Temperature

CASE

PENNSTATE

UIC

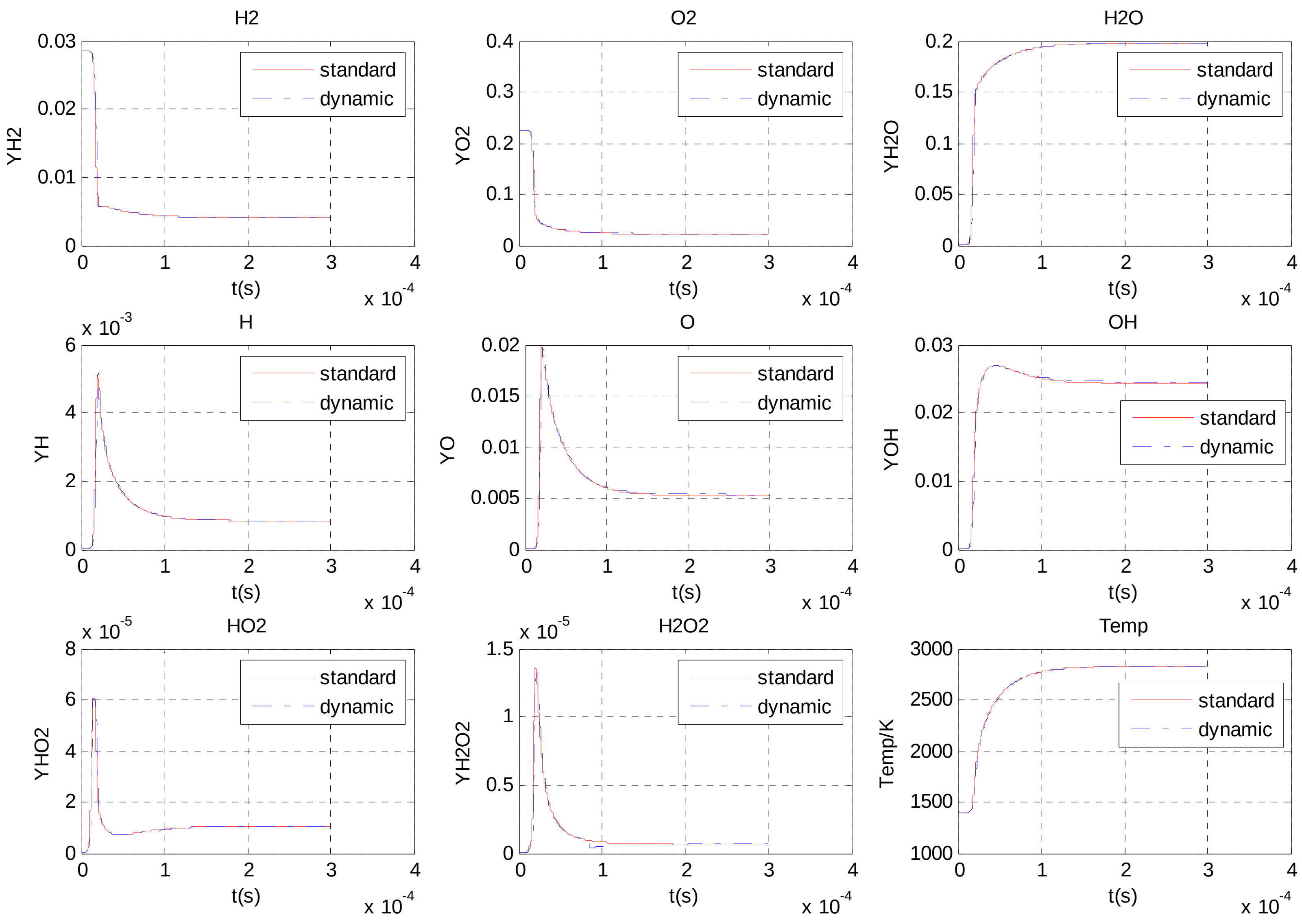
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

4. A Dynamic Multi-Scale (DMS) Kinetic Reduction Model

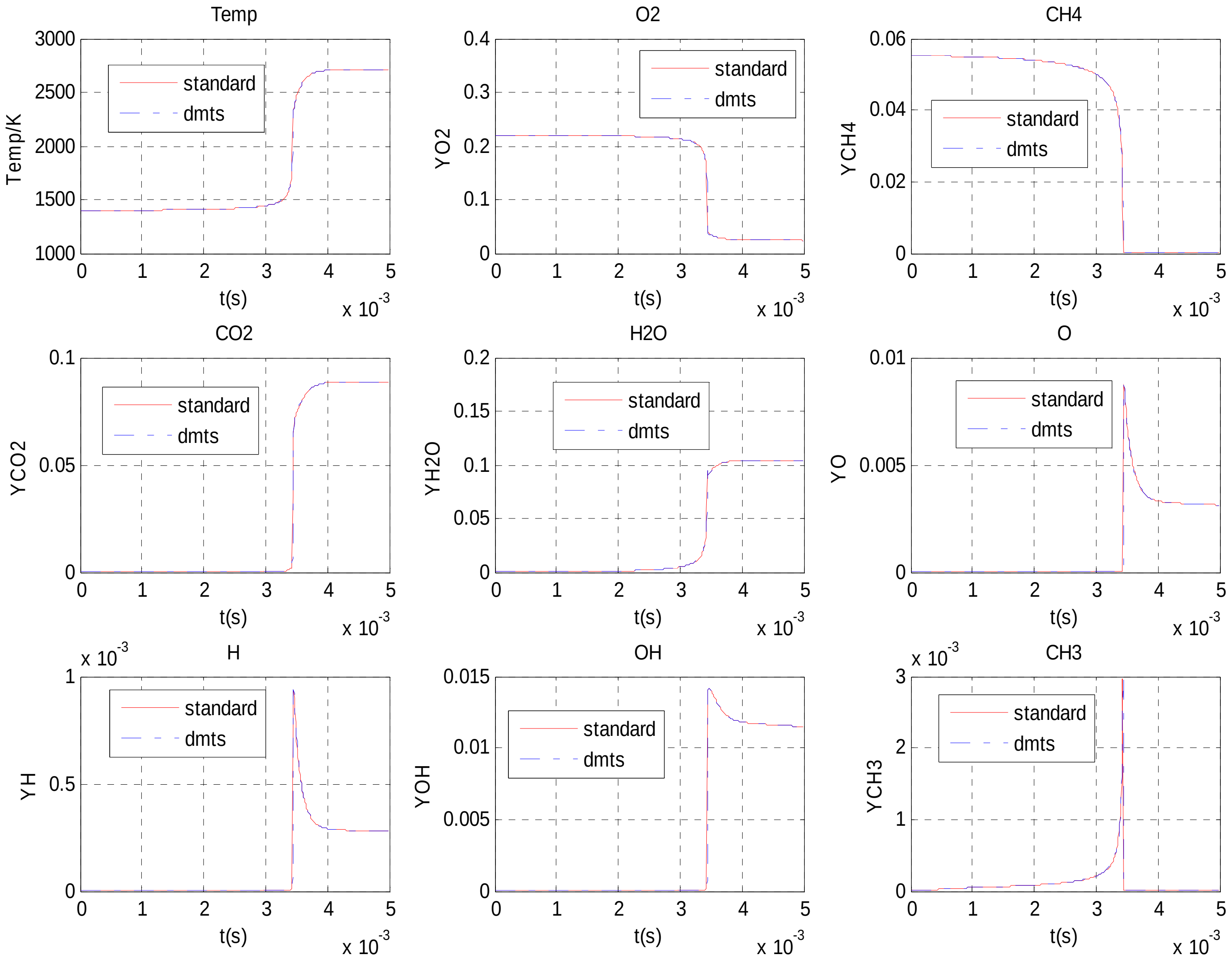
Time scales in reactive flow

Chemical time		Physical time	
	1 s		
NO formation	10^{-2}s	Flow time	
Product formation H2O	10^{-4}s	Transport time Molecular Turbulent	Physical interest
Radical formation H	10^{-6}s		
	10^{-8}s	Radiation transfer quasi-steady state	?
Radical formation H2O2 quasi-steady state?	10^{-10}s		DNS Time-step

Validation of DMS Method (Hydrogen)



Validation of DMS Method (Methane)



Further Kinetic Mechanism Reduction: A Path Flux Analysis Method

Reaction path coefficients

$$r_{AB}^{P} \equiv \frac{A \to B}{\max(A \to X, X \to A)}$$

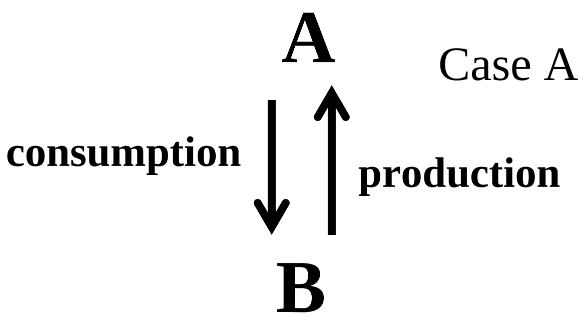
$$r_{AB}^{C} \equiv \frac{B \to A}{\max(A \to X, X \to A)}$$

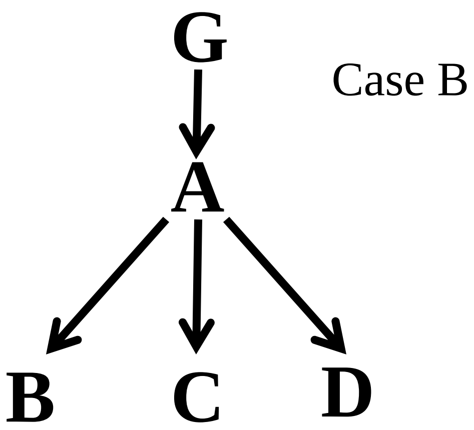
MPA: Bendtsen 2001

DRG: Lu & Law, 2005

DRG-EP: Pitsch, 2008

Reaction path

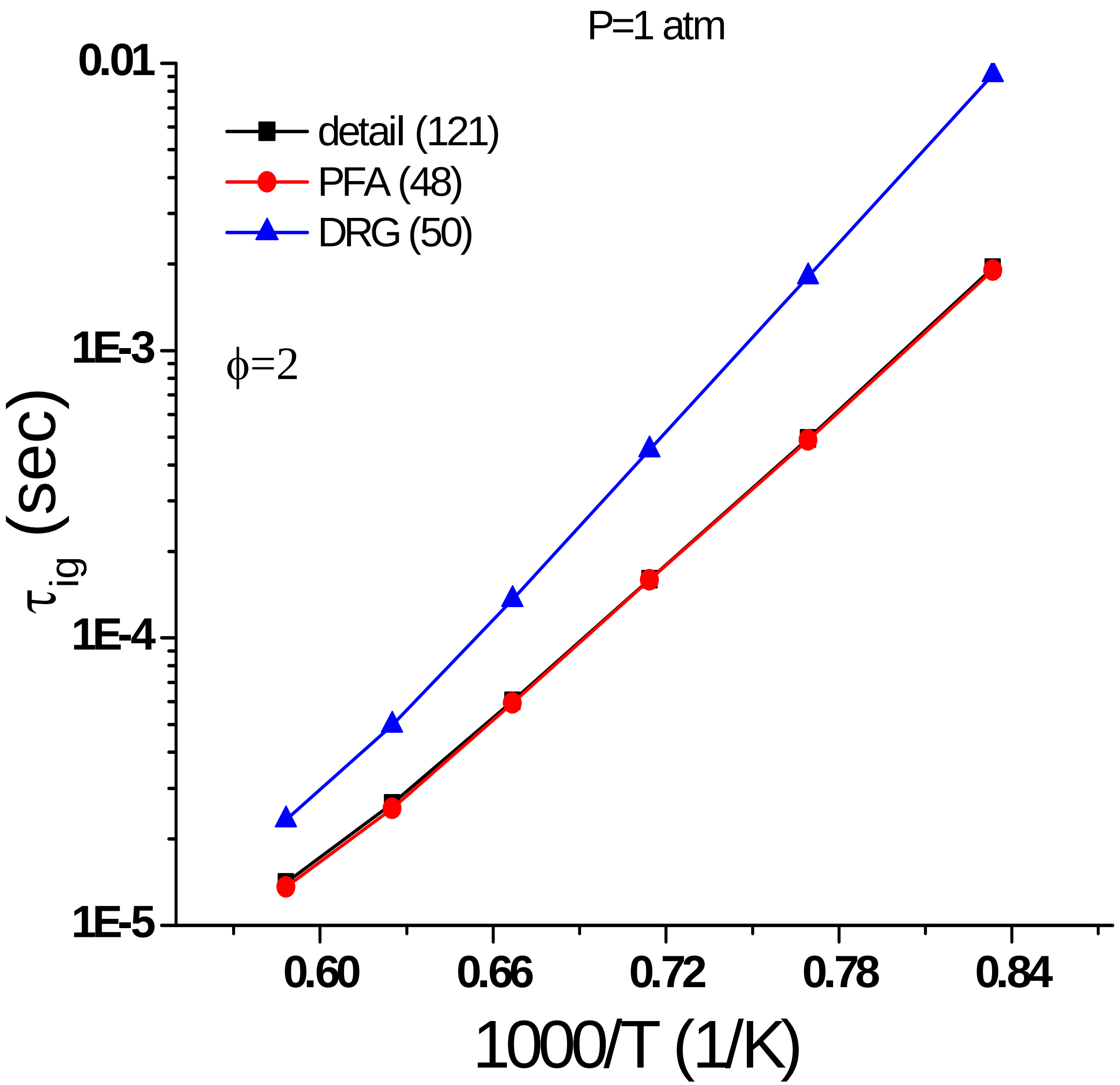




CASE PENNSTATE UIC

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
UNITED STATES AIR FORCE

Results and Comparisons on n-Decane Ignition



Conclusions

- The extinction limits of 1,3,5 and 1,2,4 trimethy-benzenes are much narrower than toluene and n-decane. Blending of aromatics in alkanes can effectively control the extinction limit of surrogate fuel components.

- The extinction limit of toluene blended n-decane is found linearly dependent on the maximum OH concentration. The OH concentration is controlled by the kinetic coupling between aromatics and alkanes.

- Transport affects extinction limit in both thermal and kinetic ways via major species and active radicals.

- The soot volume fraction increases with the concentration of toluene. The measured soot volume fraction by LII agrees well with the TSI prediction. These linear dependences on aromatics blending level provide a convenient way to construct surrogate models.

- A dynamic multi-scale model and a P-MARS mechanism reduction model are developed.