Characterization of Extinction Limits of Nonpremixed Counterflow Flames: Effect of Boundary Conditions

with fuels H2(diluted), CH4, C2H4, C3H6, n-C4H10

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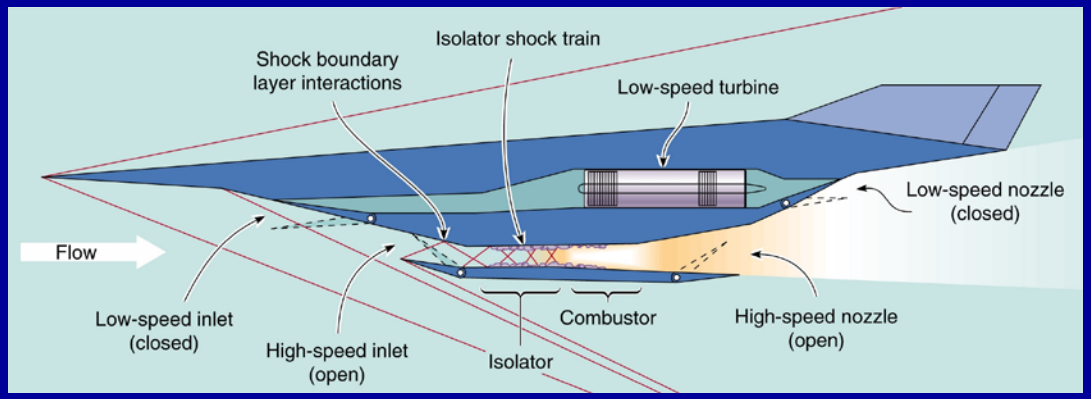
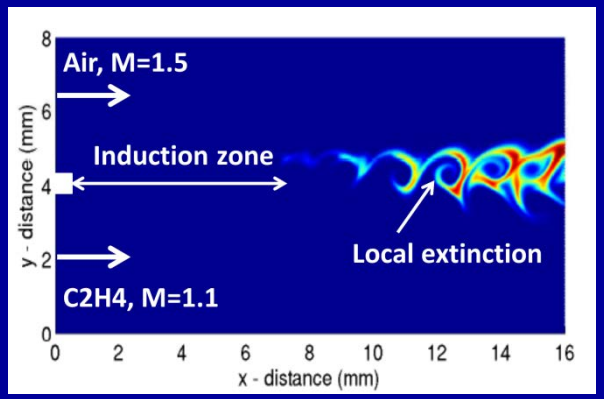
AFSOR-NASA National Center for Hypersonic Combined Cycle Propulsion

MACCCR Fuels Meeting, September 21, 2011

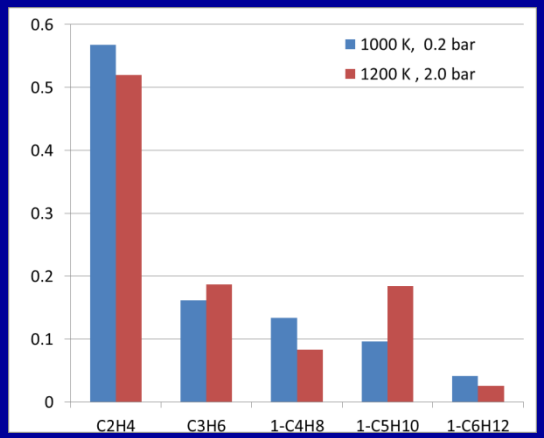
Background/Objectives

- **Reduced-order kinetic models for hypersonic reacting flow simulations**

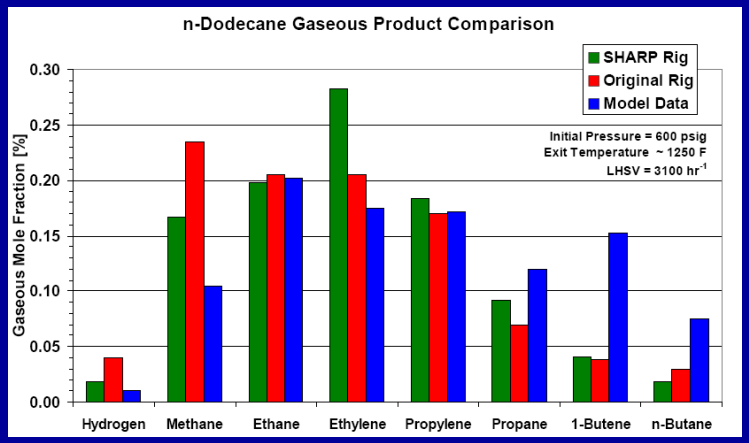




- **Fuels of interest: pyrolyzed fuel components (H2, CH4, C2H4, …)**



Heptyl radical decomposition from **NIST** shock tube studies, for 1000-1200 K and 0.2-2.0 bar



n-dodecane decomposition in a tube flow reactor investigation at **UTRC**

Background/Objectives (cont.)

Skeletal and Reduced Reaction Models:

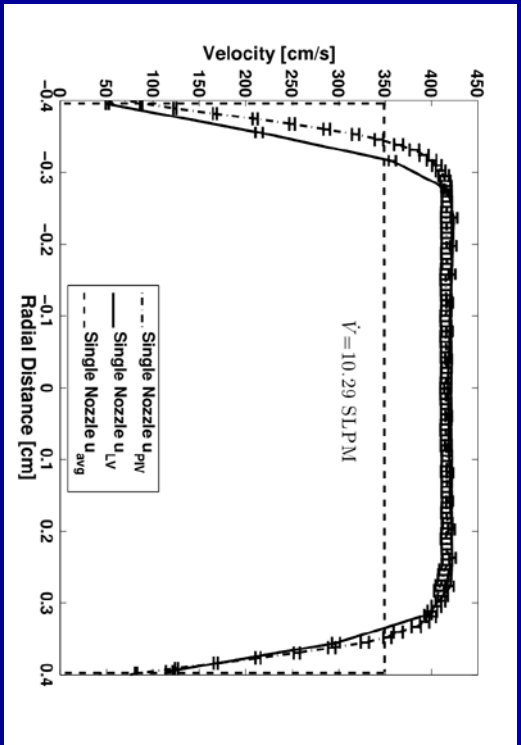
- **PCAS** based method for **ethylene-air:**
  - **38 species skeletal model** from USC Mech II* (2009)
  - covers ignition, propagation, and **extinction**
  - *Esposito and Chelliah. Combustion and Flame 158 (2011)*
- **QSSA** for reduced reaction model for ethylene-air:
  - **20-step reduced reaction model**
  - *Zambon and Chelliah, Combust. and Flame (2007)*
- The skeletal and reduced models developed have been shared with Center members, NASA, AEDC, AFRL, GE, and others

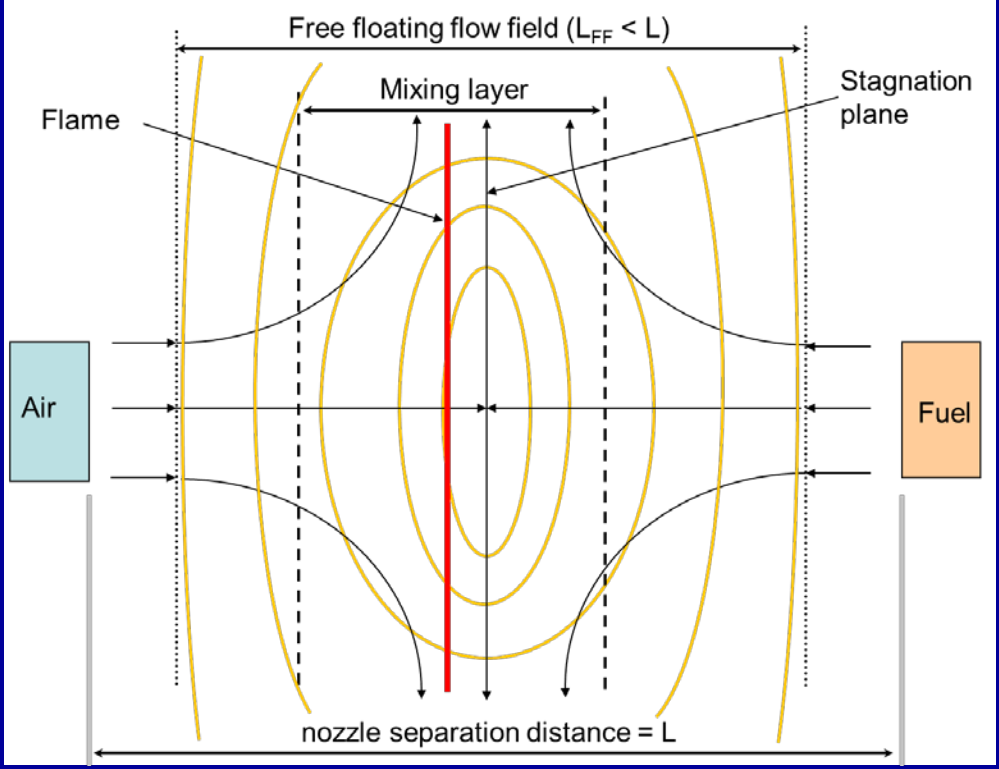
Accuracy of detailed kinetic model in prediction extinction: Focus of this presentation!

The Hypersonic Propulsion Center will clearly benefit from the work done by this group!!!

Boundary Conditions

- **What is the ideal nozzle separation distance?**
- **What is the role of boundary conditions (BC)?**
- **In experiments, BC's depends on L/D (separation distance/diameter)!**
- **In quasi one-dimension numerical simulations – D has no role!**





$L_{FF}<L$

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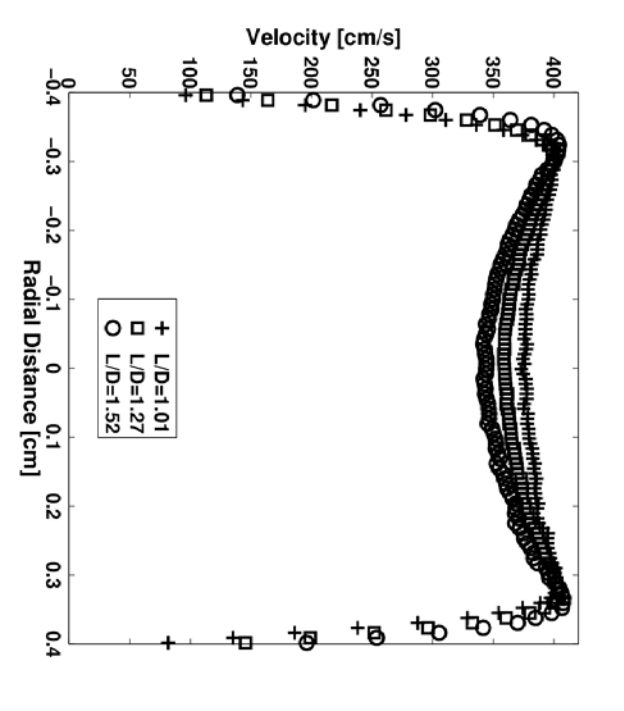

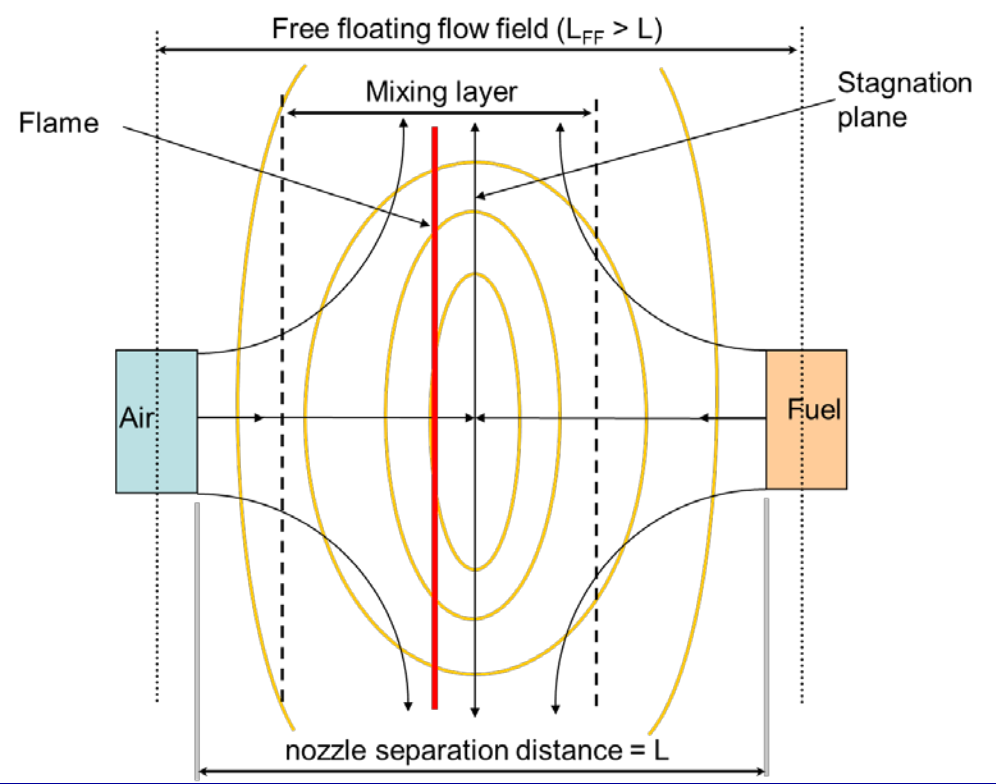

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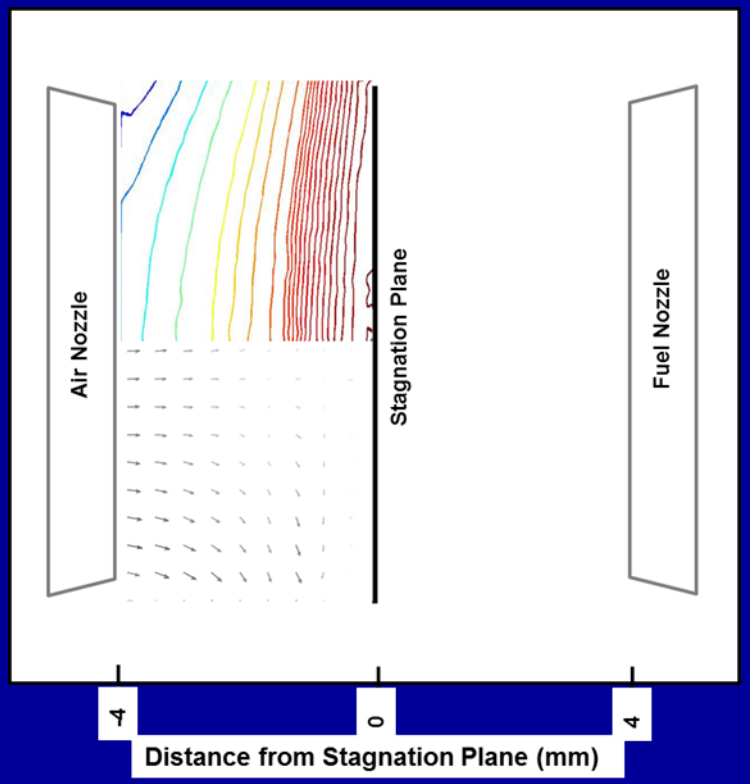
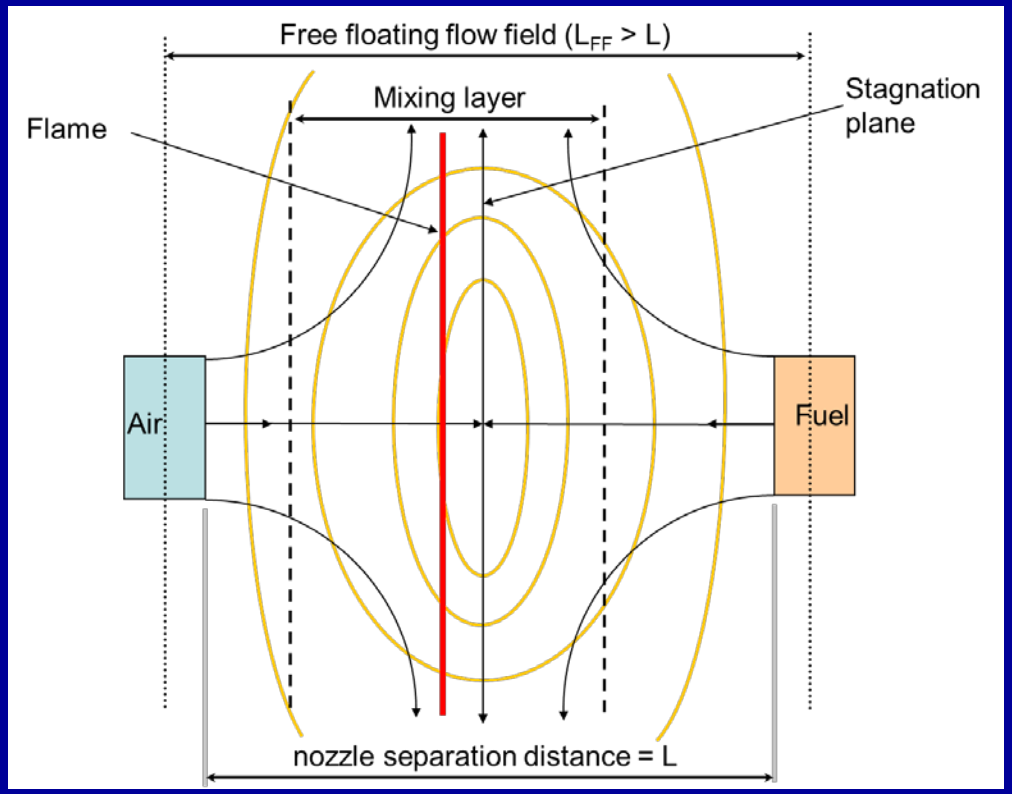
Pressure contours from PIV data





$L_{FF}>L$

Few Definitions

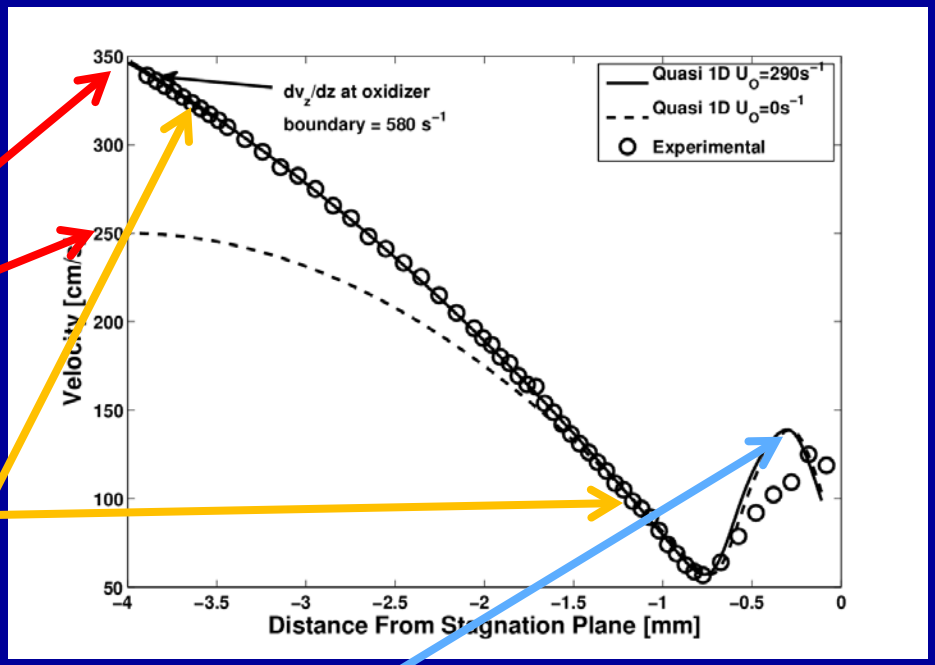
- **Extinction strain rate (s^{-1})**
  - ***Global extinction strain rate*** *(with momenta balanced), Seshadri and Williams, 1978*

$$a_{global} = \frac{4u_{air}}{L}$$

  - *Local extinction strain rate*

$$a_{local} = \left(\frac{du}{dx}\right)$$

  - *Local extinction strain rate however is influenced by inflow velocity gradient* $\frac{du}{dx} = 2U$



Chelliah et al. (1990), Sarnacki et al. (2011), and others

- **Scalar dissipation rate (s^{-1})**

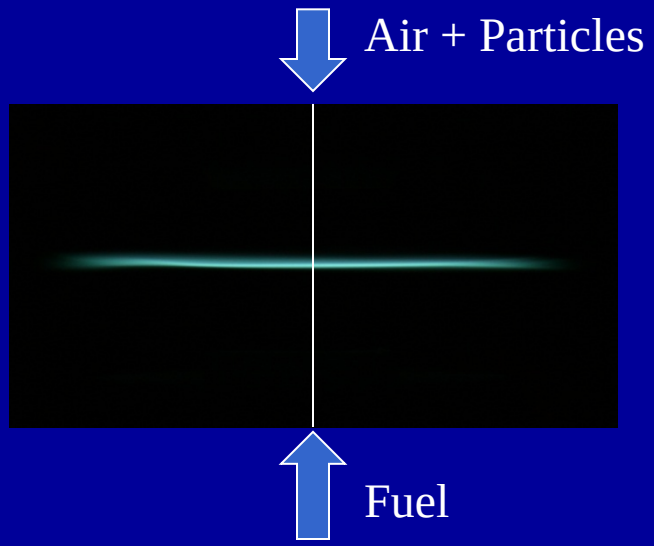
$$\chi_{st} = 2\frac{\lambda}{\rho c_p}\left|\frac{dZ}{dx}\right|^2$$

- Completely independent of the outer flow description!
- Can we measure it accurately???

Measurement Uncertainties

- **Velocity:** uncertainty of local velocity measurement (typically1-3%) --- slip, LV/PIV, standard error of the sample mean (SEM)

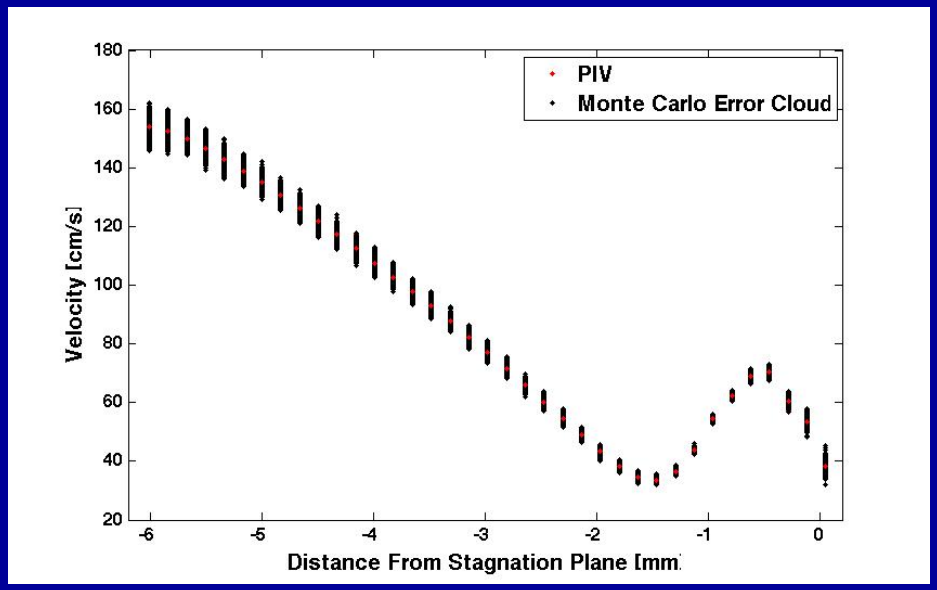
$$\Delta u_{TOT} = \sqrt{(\Delta u_{slip})^2 + (\Delta SEM)^2 + (\Delta u_{LV})^2}$$



- **Strain rate:** uncertainty of the estimated local strain rate --- (i) regression fit and (ii) repetition

$$s_{tot} = \alpha \sqrt{(s_{reg})^2 + (s_{rep})^2}$$

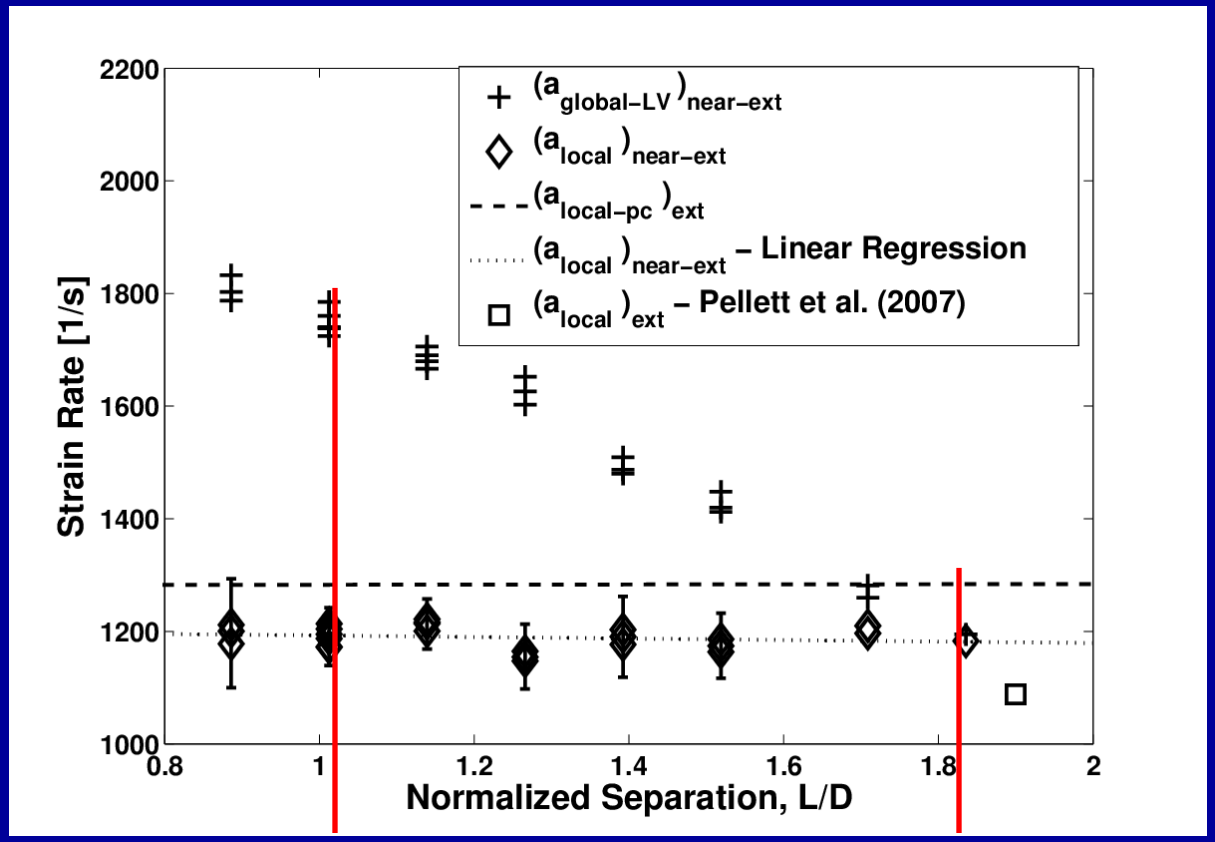
  - Used a MC approach based on 1000 normally distributed random points
  - Regression and repeatability had nearly equal contribution to the total uncertainty



Results - Experimental

- Global vs. local extinction strain rate as a function of L/D

Ethylene-air Non-premixed Flames



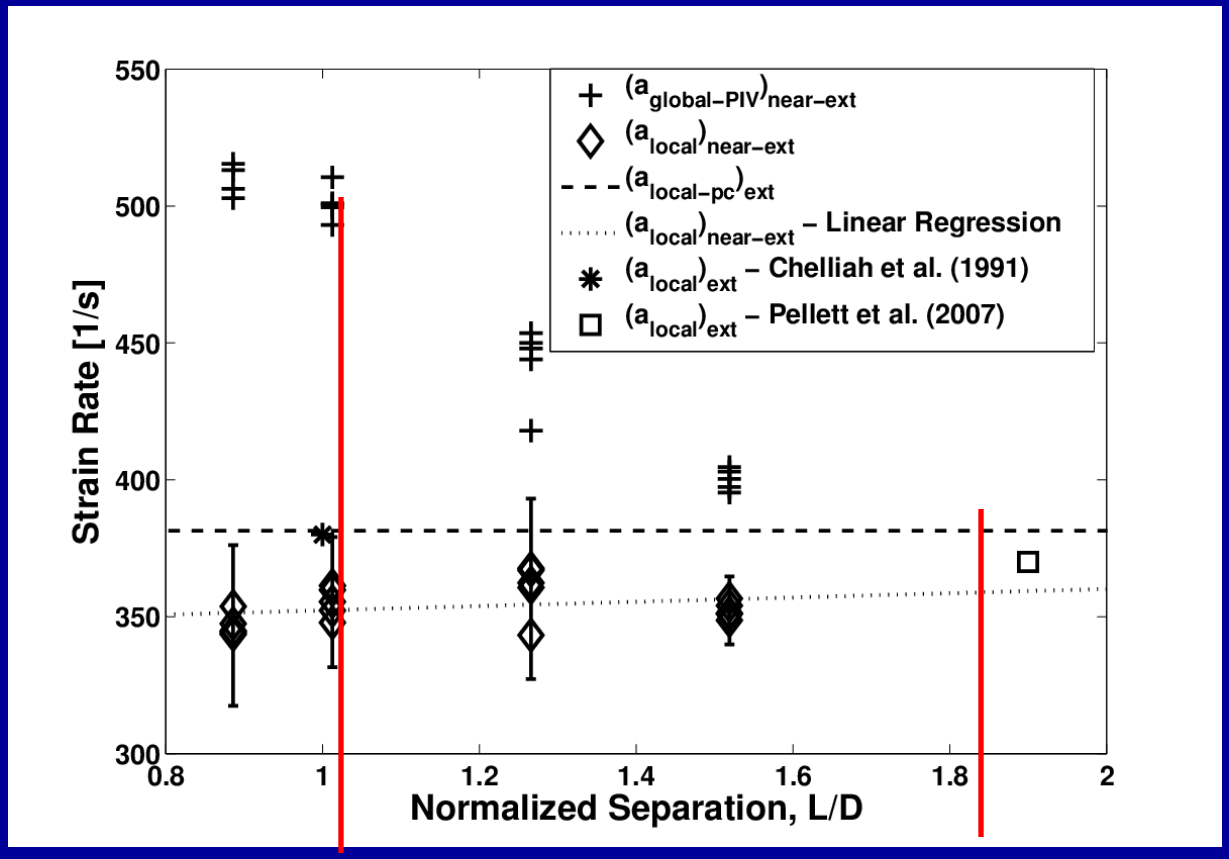
L/D~1.0($L<L_{FF}$)
U = 290 s^{-1}

L/D~1.8($L=L_{FF}$)
U = 0 s^{-1}

Results - Experimental

- Global vs. local extinction strain rate as a function of L/D

Methane-air Non-premixed Flames



L/D~1.0($L<L_{FF}$)
U = 112 s^{-1}

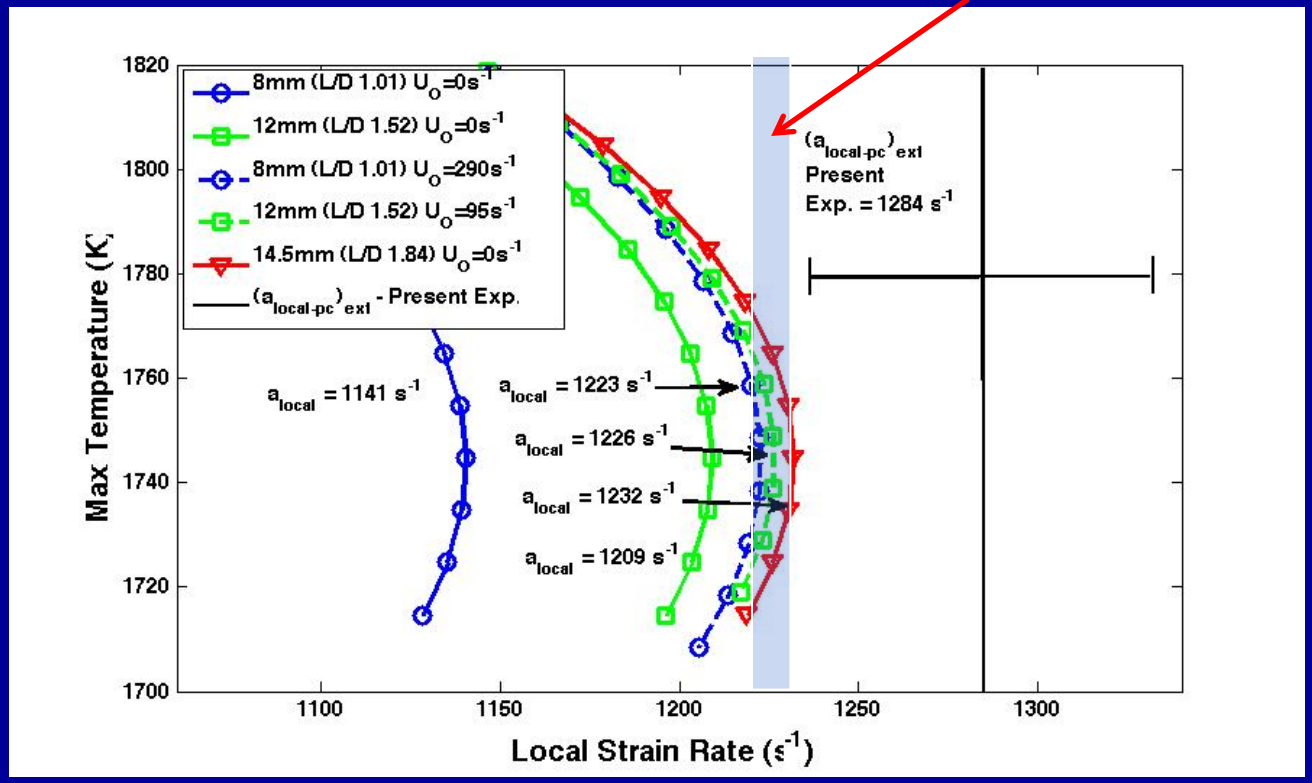
L/D~1.8($L=L_{FF}$)
U = 0 s^{-1}

Results – Numerical Predictions

- Quasi 1D formulation (Kee et al. (1988), Smooke et al. (1990))
- **For $L<L_{FF}$, must use $U\neq 0$ bc's; for $L=L_{FF}$, $U=0$ is fine (plug flow bc); for $L>L_{FF}$ quasi 1D formulation cannot be used!**
- Can one find L_{FF} without LDV/PIV? Probably not!
- ***U* from experiments for a range of *L*:**

  $\Rightarrow$ Predicted extinction strain rate has an uncertainty based measured *U*!

<u>Ethylene-air</u> extinction curves predicted using USC Mech II*(JetSurf 1.0)

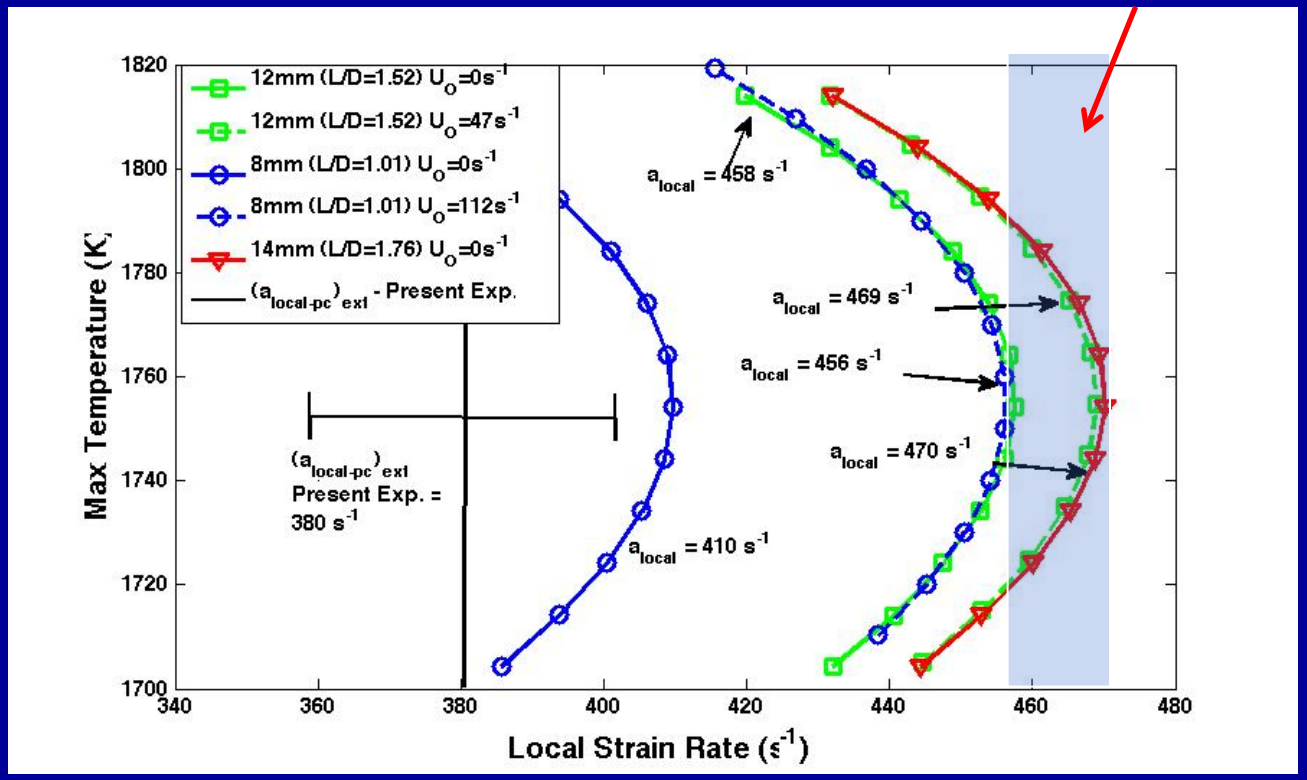


Results – Numerical Predictions

- Quasi 1D formulation (Kee et al. (1988), Smooke et al. (1990))
- **For $L<L_{FF}$, must use $U\neq 0$ bc's**; for $L=L_{FF}$ use $U=0$ is fine; for $L>L_{FF}$ quasi 1D formulation cannot be used!
- How do you find L_{FF}???
- Use ***U* from experiments for a range of *L***

  $\Rightarrow$ Predicted extinction strain rate has an uncertainty based measured *U*!

Methane-air extinction curves predicted using USC Mech II*(JetSurf 1.0)



Summary of Experiments and Predictions

Fuel-air system	Local Extinction Strain Rate (s^{-1})	Model Predict. (s^{-1}) with finite U's	Scalar Dissipation Rate, χ_{st} (s^{-1})
Methane	380±21	456-470	16.6
Ethylene	1284±48	1223-1232	-
Propylene	617±34	606-624	-
n-Butane	499±38	544-550	-

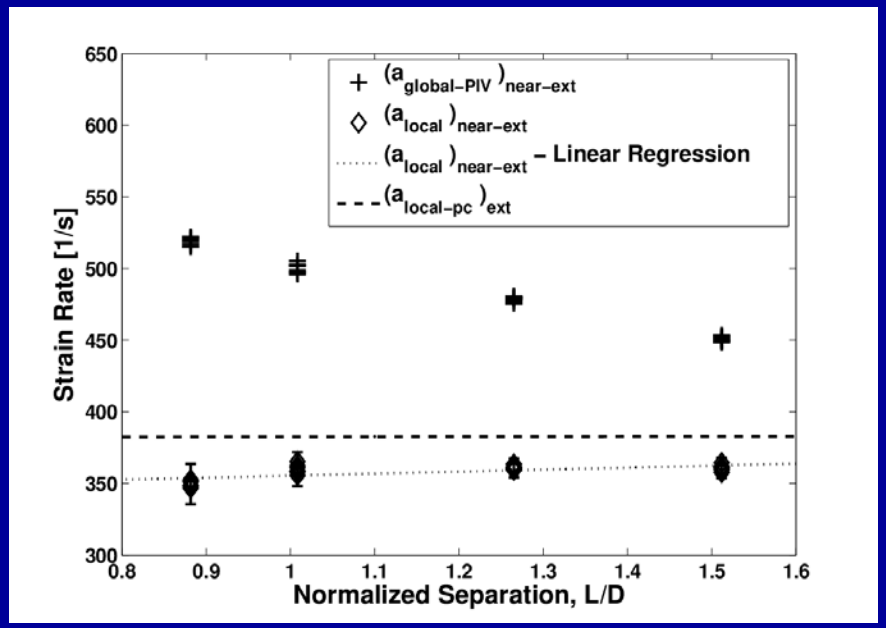
- Sheen et al. (2009) USC MechII* model, optimized for ethylene works well for ethylene-air non-premixed extinction limit, but not so for methane-air extinction!

- **Full details can be found in Sarnacki, Esposito, Krauss, and Chelliah, to appear in *Combust. and Flame*.**

The story doesn't end here!!!

What About Nozzle Diameter?

- Previous data were using D=**7.9mm set of nozzles** with an area ratio of 24
- Experiments were repeated with D=**14.5mm set of nozzles** for methane



Fuel-air system	a_{ext} from expermnt.	a_{ext} from model	(χ_{st}) from model
Methane D=7.9 mm	380±21	456-469	16.6
Methane D=14.5mm	383±13	487-504	16.6

↑

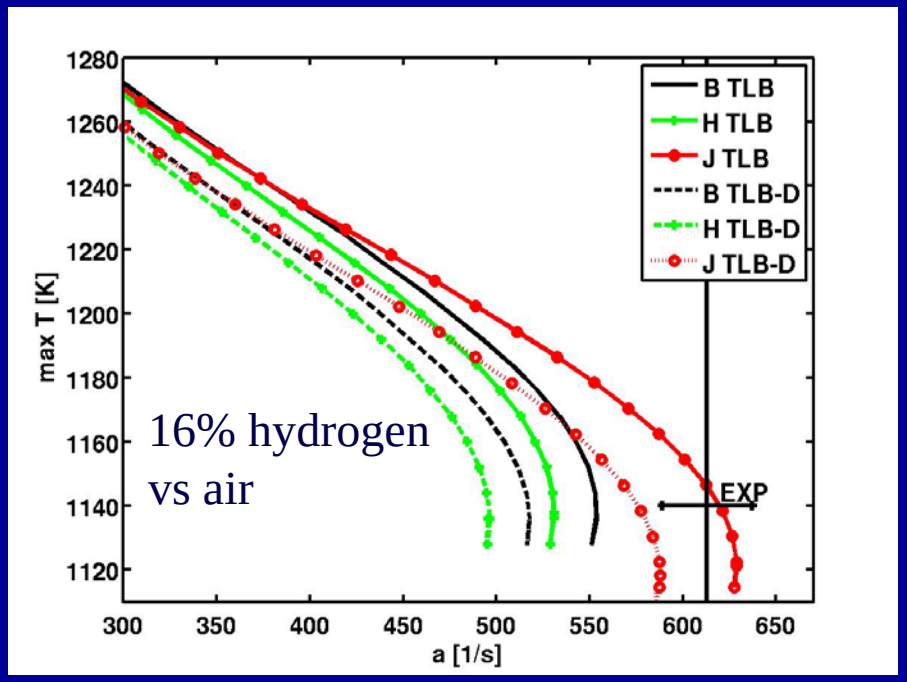
~30s^{-1} different!!!

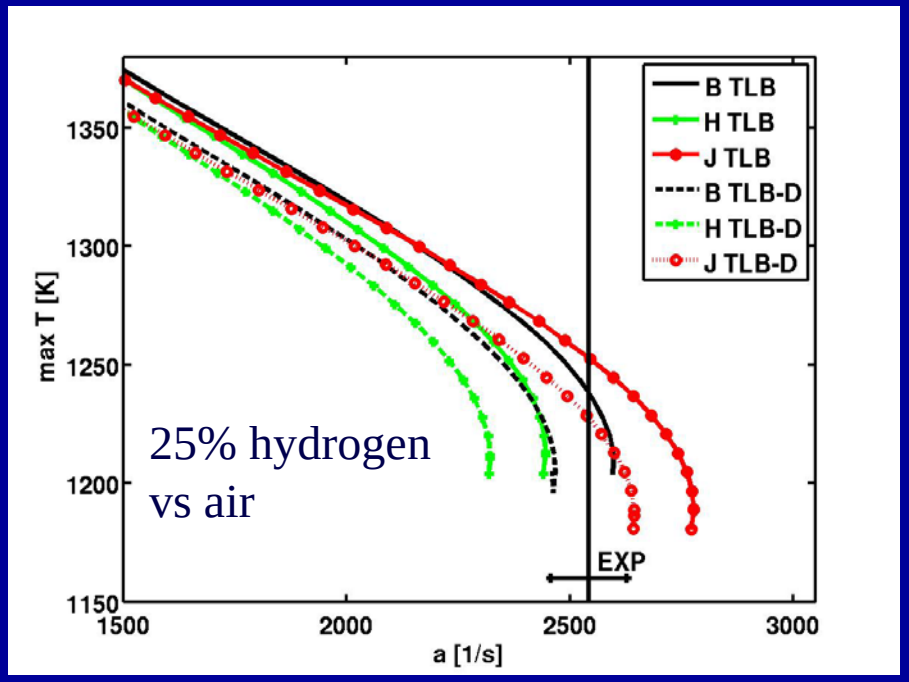
- Note: D is not an input in quasi one-dim. model; can only prescribe L and U!
- **<u>Need to repeat above experiments with identical area ratio nozzles?</u>**
- **<u>Full 2D simulations?</u>**

--- happy to provide all the experimental data!

What About Transport Coefficient Uncertainties?

- The best system to address this issue is via **hydrogen flames**
- Undiluted hydrogen-air has a very high extinction strain rate (~8000 s^{-1})
- Used diluted-hydrogen in air AND diluted-hydrogen in diluted-air





- **Three kinetic models:**
  - Hong et al. (2011), Burke et al. (2011), JetSurf2.0* (2011)
- **Two transport:** Tranlib and modified Tranlib fits from Middha et al. (2002)
- Detailed paper will be presented at ***ESS Meeting at Hartford, Oct. 2011***

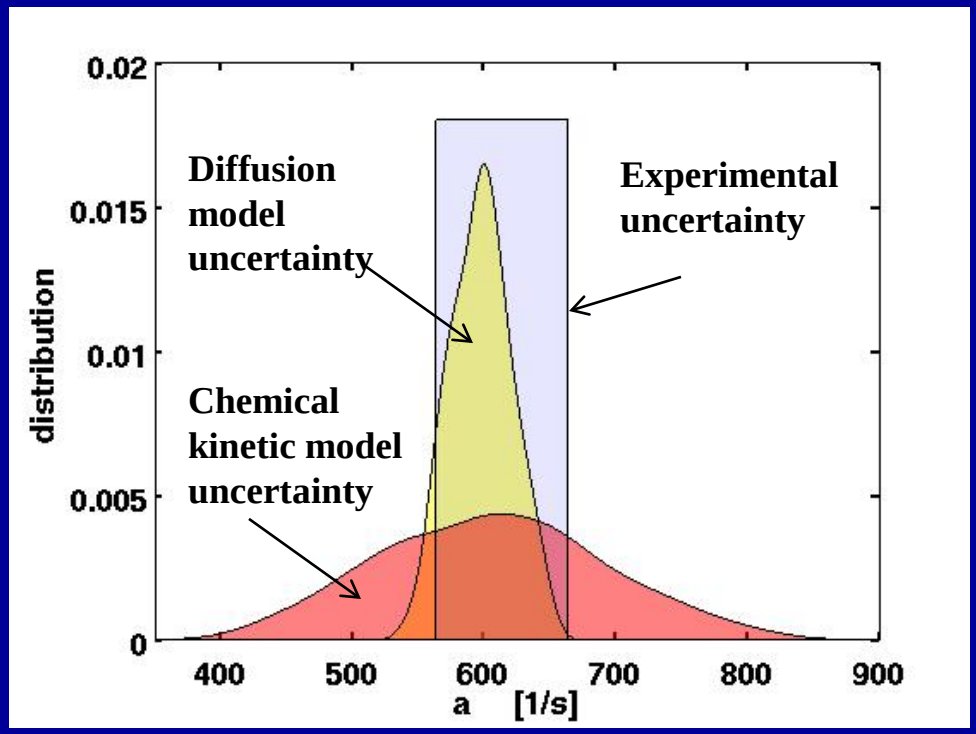
Comparison of Sensitivities

- Global sensitivity analysis of **<u>kinetic and transport coefficient uncertainties</u> in predicting diluted-hydrogen and air flame extinction**
- Sensitivity coefficients from MC simulation of top 1% of binary diffusion coeff. (Using TeraGrid)

$D_{i,j}$	$S_i^{(A)}$	$S_i^{(B)}$
H_2, N_2	0.48	0.72
H, N_2	0.43	0.16
O_2, N_2	0.05	0.08

- Sensitivity coefficients from MC simulation of top 1% CK parameters.

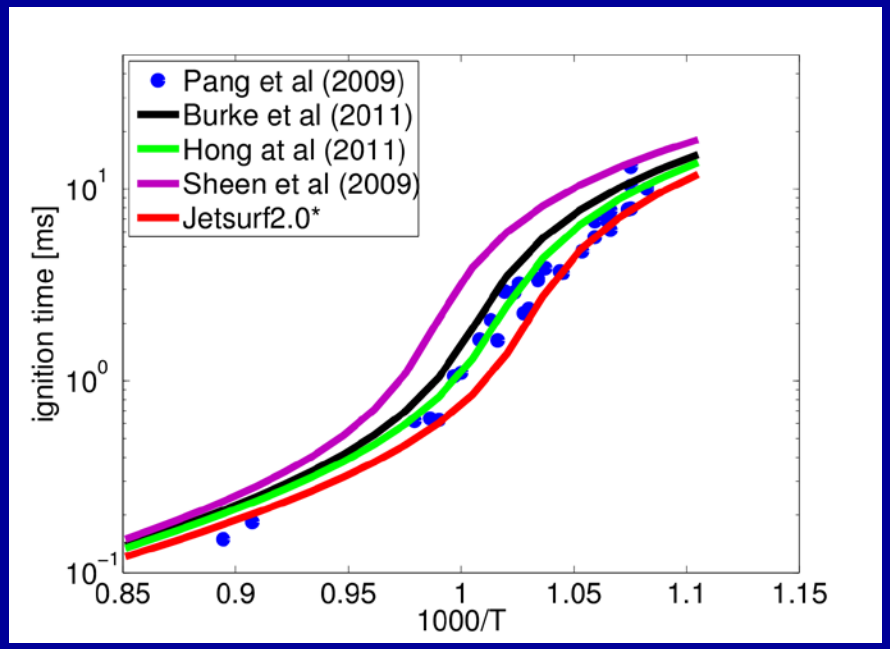
Reaction	S_i
(R1) $HO_2+H \leftrightarrow 2OH$	0.37
(R2) $OH+H_2 \leftrightarrow H+H_2O$	0.29
(R3) $O+H_2 \leftrightarrow H+OH$	0.11
(R4) $H+O_2 \leftrightarrow O+OH$	0.12
(R5) $OH+HO_2 \leftrightarrow H_2O+O_2$	0.03
(R6) $H+OH+M \leftrightarrow H_2O+M$	0.03



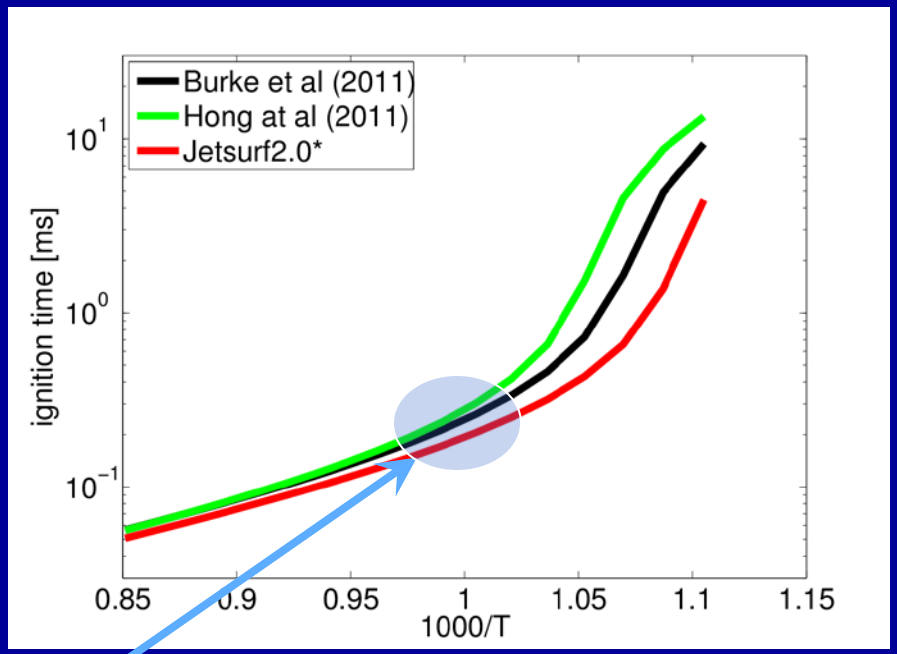
Diluted hydrogen and air extinction strain rate distribution due to model uncertainties

How about Ignition Delay Predictions?

- In hypersonic flow fields, accurate prediction of **ignition delay is critical!.**
- Ignition delay predictions using several hydrogen kinetic models:



Comparison with experimental ignition delay data of H2/air from Pang et al. (2009) at p=3.5atm, ϕ=1.0, in Ar



Comparison of ignition delay predictions at p=1 atm, ϕ=1.0 in air

Trends are consistent with <u>extinction limit predictions</u>!!!

Comparison of Hydrogen Models

National Institute of Standards and Technology

NIST CHEMICAL KINETICS MODEL DATABASE

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Results 1 - 24 of 24 **Search In:** All Models **PreExp units:** mole **Energy units:** cal **Sort by:** Rank

View	Reaction	Class [Sites]	log(Ratio)	A	b	E	Datatype	Reference	Model	Kinetics DB
1	H2O2 + H = OH + H2O	O-H+H [O-O]	-0.4	1.02E+13	0.00	3577			2011-HOx-Hong	Fwd Rev
2	H2O2 + (m) = OH + OH + (m)	O-O [OH/OH]	0.1	8.59E+14	0.00	48560			2011-HOx-Hong	
3	H2O2 + H = HO2 + H2	O-H+H [O-O]	-0.5	1.21E+07	2.00	5200			2011-HOx-Hong	Fwd Rev
4	H2O2 + O = HO2 + OH	O-H+O [O-O/O:]	1.2	8.43E+11	0.00	3970			2011-HOx-Hong	Fwd Rev
5	HO2 + H = O2 + H2	O.O-H+H	-0.1	3.66E+06	2.09	-1450			2011-HOx-Hong	Fwd Rev
6	O2 + (m) + H = HO2 + (m)	O.O-H (-)	-0.3	5.59E+13	0.20	0			2011-HOx-Hong	
7	HO2 + O = O2 + OH	O.O-H+O	0.3	1.63E+13	0.00	-445			2011-HOx-Hong	Fwd Rev

Conclusions

- Effects of **inflow boundary conditions**, **seed particles**, **measurement uncertainties** on non-premixed flame extinction limits were carefully analyzed, for a range of fuels (H2, CH4, C2H4, C3H6, n-C4H10)
- **Local extinction strain rate** was found to be **nearly invariant** with the nozzle separation distance (**L**), for two sets of nozzles used
- **Axial Velocity gradient** at the nozzle exit was shown to be a function of nozzle separation distance, nozzle diameter, (or nozzle shape?), and fuels used.
- In quasi one-dimensional simulations, implementation of **experimentally measured boundary conditions is critical for $L<L_{FF}$**
- **Uncertainty analysis** of both **kinetics and transport parameters**, based on Morris Method and full Monte Carlo Methods are continuing using the TeraGrid and will provide guidance to focus on a subset of parameters for future investigations