Flame Studies of Jet Fuels and Surrogate-Related Neat Components

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MULTI AGENCY COORDINATION COMMITTEE FOR COMBUSTION RESEARCH (MACCCR) FUELS RESEARCH REVIEW

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Technical Monitor: Dr. Julian M.Tishkoff

General Objectives

1. **To determine experimentally accurate archival fundamental flame properties (ignition, propagation, extinction) for:**
   - **Selected jet fuels**
   - **Single-component hydrocarbons**
   - **Mixtures of chosen hydrocarbons**

2. **To model experiments using detailed description of chemical kinetics and molecular transport.**

3. **To provide insight into the chemical and physical mechanisms that control the flame response of large (liquid) hydrocarbon flames.**

Objectives of Year 1

1. **To determine experimentally laminar flame speeds and extinction states of atmospheric pressure flames of:**
   - **C_5-C_{12} *n*-paraffins**
   - **JP-8**

2. **To assess the relative importance of kinetics versus molecular transport on the measured flame properties.**

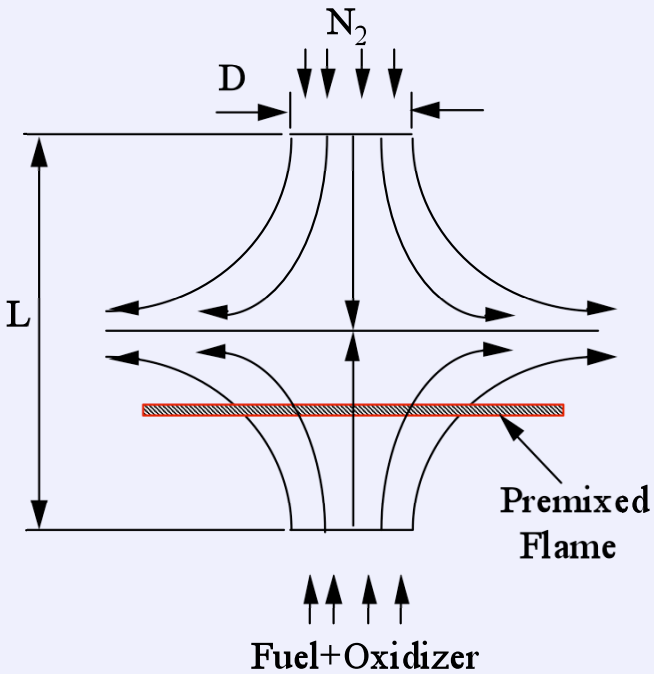
Challenges

1. **For these large molecular weight fuels the vapor pressure is low. Performing pre-vaporized fuel experiments requires:**
   - **Significant heating to create the vapor. The heating process could thermally crack the fuel.**
   - **Small residence times, which, however, tend to be large, i.e. few seconds to several minutes in flame experiments; extent of thermal cracking depends on time as well.**
   - **Elimination of cold spots throughout the reactant path to avoid fuel condensation.**
2. **As pressure and fuel molecular weight increase, those issues are notably more profound to the point that could render experiments unreliable/unfeasible**
3. **The large molecular weight discrepancy between fuel and oxidizer can complicate experimental data interpretation, especially when measurements are not direct and data processing is required. Knowledge/experience acquired from gaseous fuel flames may not be adequate.**

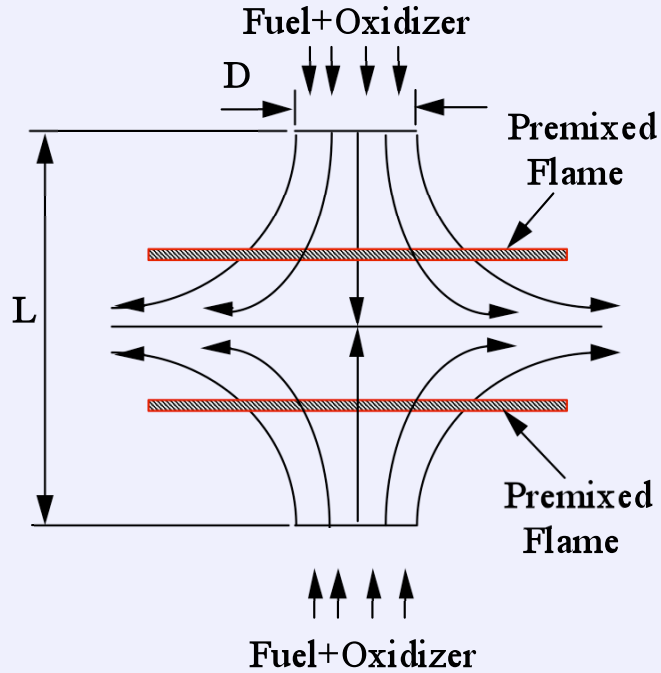
Experimental Approach - General

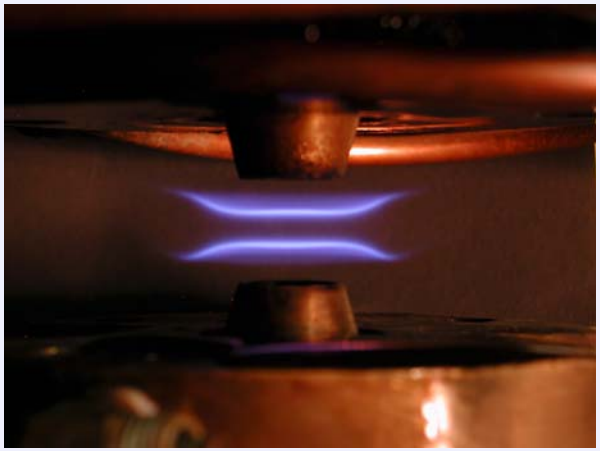
- **Use of counterflow technique (L/D ≤ 1)**

Single-flame configuration



Twin-flame configuration

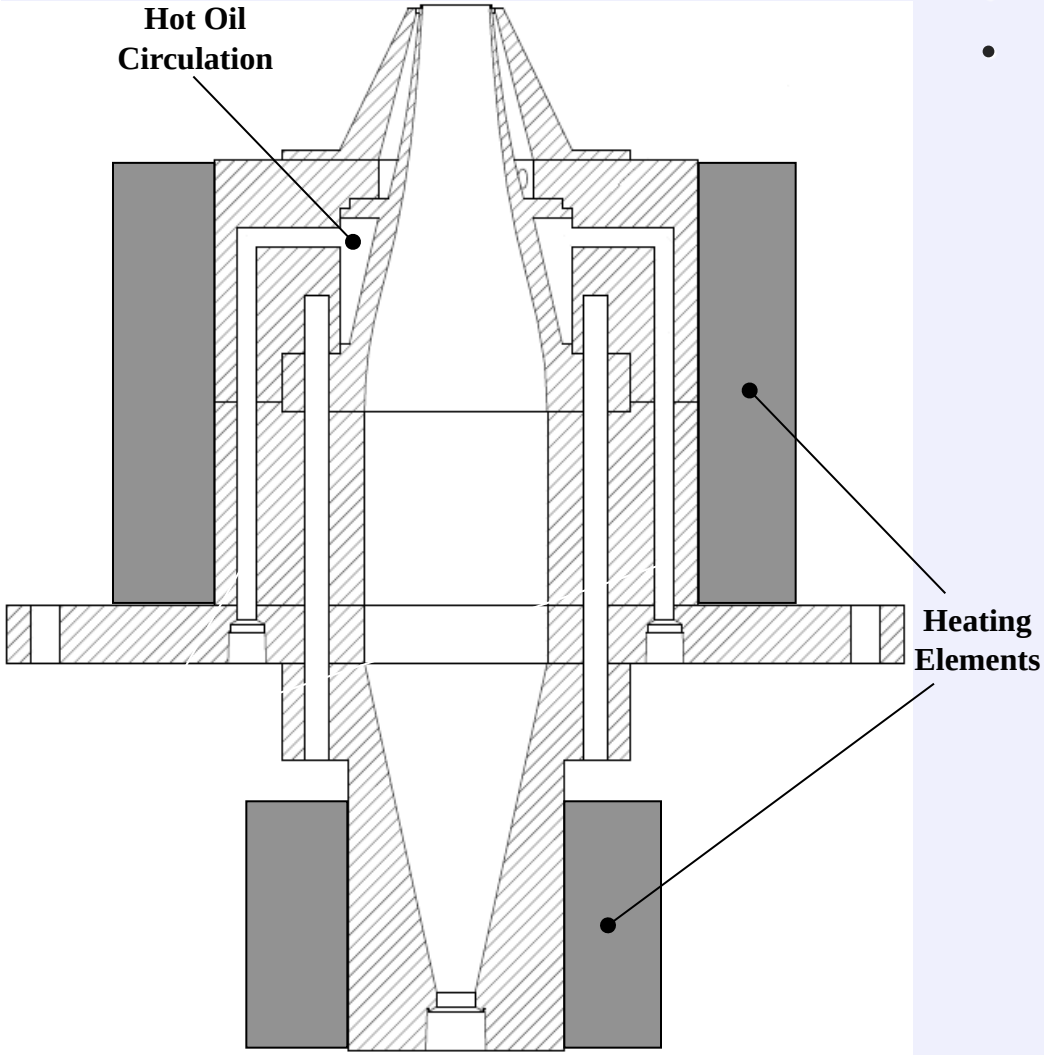




- **Pressure chamber:**
  - **Pressure range 1-10 atm**
- **Diagnostics:**
  - **Laser Doppler Velocimetry (LDV)**
  - **Digital Particle Image Velocimetry (DPIV)**
  - **Thermocouples**

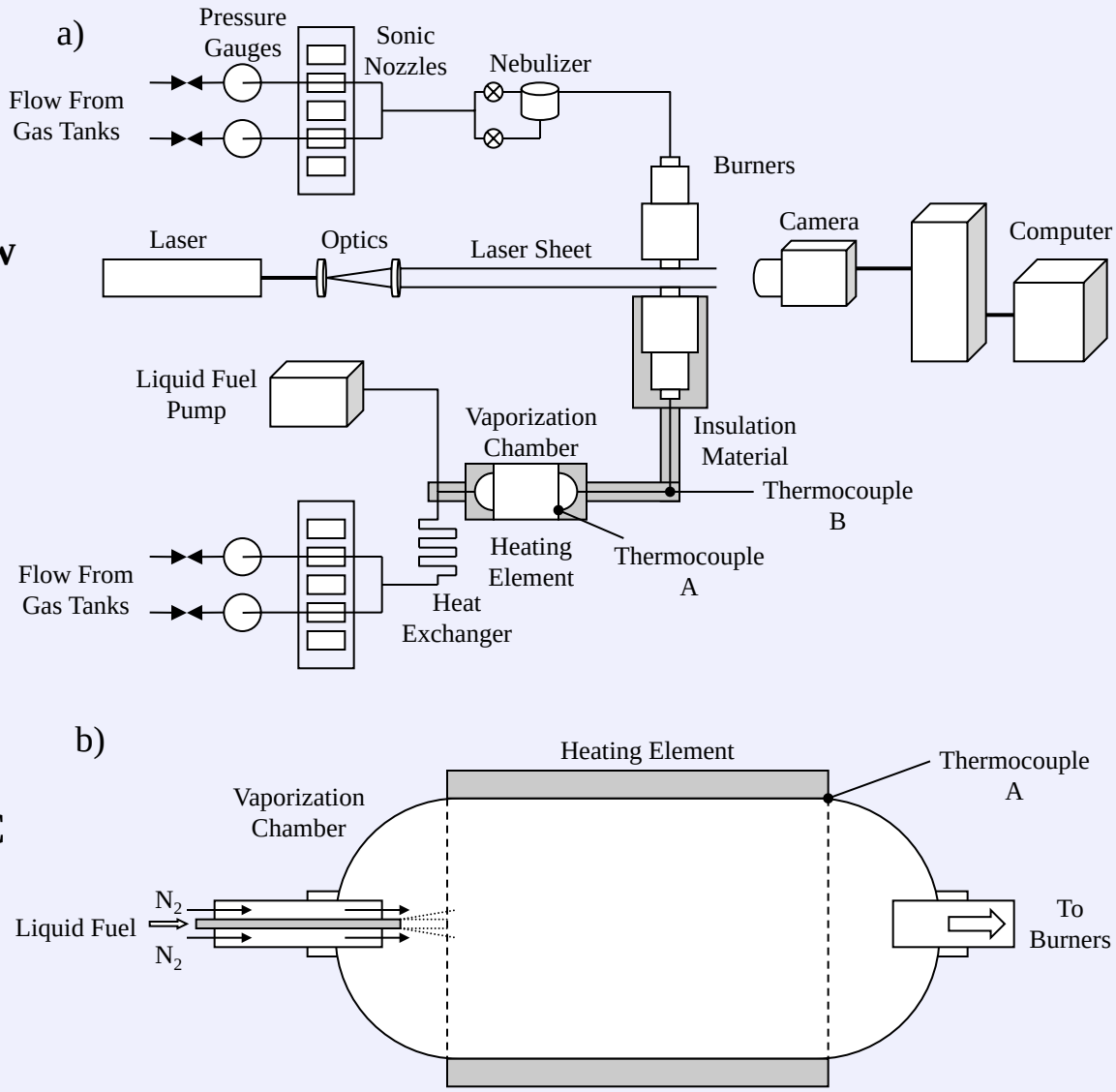
Experimental Approach – New Generation of Burners

- Capable of operating at 300°C
- Internal hot oil circulation
- Contoured to produce a flat top profile



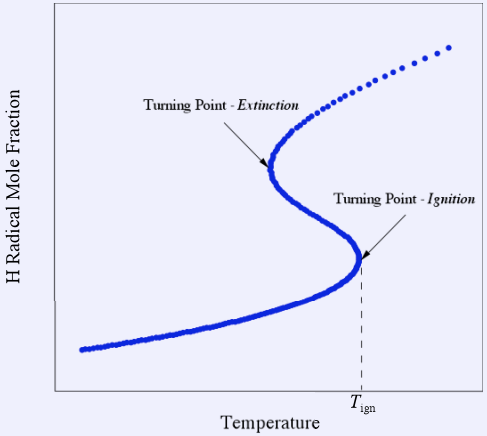
Experimental Approach - Details

- **Evaporation of the liquid fuel achieved by a liquid fuel system (based on design from Davis & Law 27th Symposium)**
- **Partial pressure of the fuel vapor kept below its vapor pressure**
- **Incoming N_2 temperature, T_{inc}: 20-200 °C**
- **Chamber wall temperature, T_W: 210-290 °C**
- **Fuel stream post-chamber temperature range, T_{pc}: 160-200 °C**
- **Fuel stream temperature range at the burner exit, T_b: 110-135 °C**



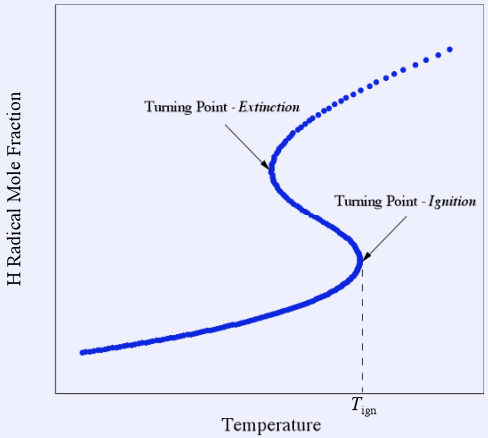
Numerical Approach: General

- Laminar flame speeds are calculated using the PREMIX code
- Extinction states are calculated using an opposed jet code modified to allow for solution around "turning-points"
- Thermal radiation for CO_2, H_2O, CH_4, and CO
- Thermo-chemical calculations are performed by:
  - CHEMKIN subroutine library
- Transport coefficients calculations are performed by:
  - Sandia Transport library updated by Wang and coworkers
- The JetSurF version 0.2 (http://melchior.usc.edu/JetSurF) kinetic mechanism developed by Wang and coworkers was implemented
  - 194 species, 1459 reactions
- Preliminary calculations performed using a mechanism by You, Egolfopoulos, and Wang (32nd Symposium) that preceded version of JetSurF version 0.2
  - 171 species, 1306 reactions



Numerical Approach: Sensitivity Analysis of All Flame Properties

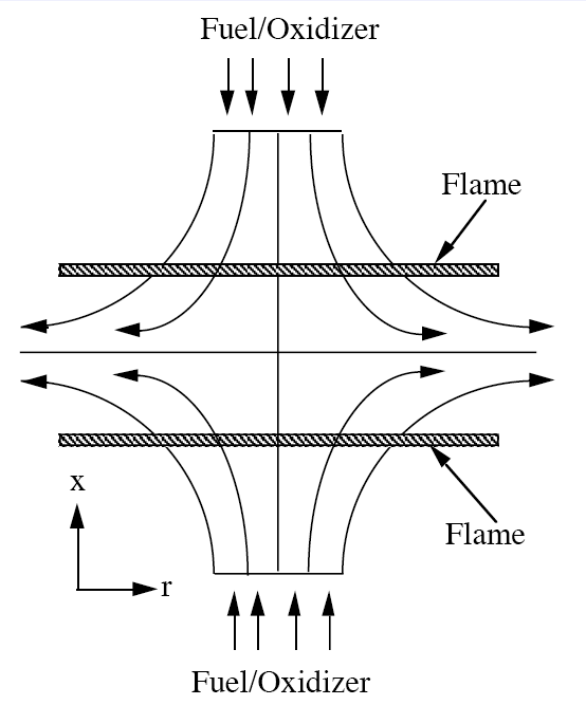
- ***Rigorous sensitivity*** **analysis can be performed now for**
  - **Laminar flame speeds**
  - **Extinction strain rates**
  - **Ignition temperatures**

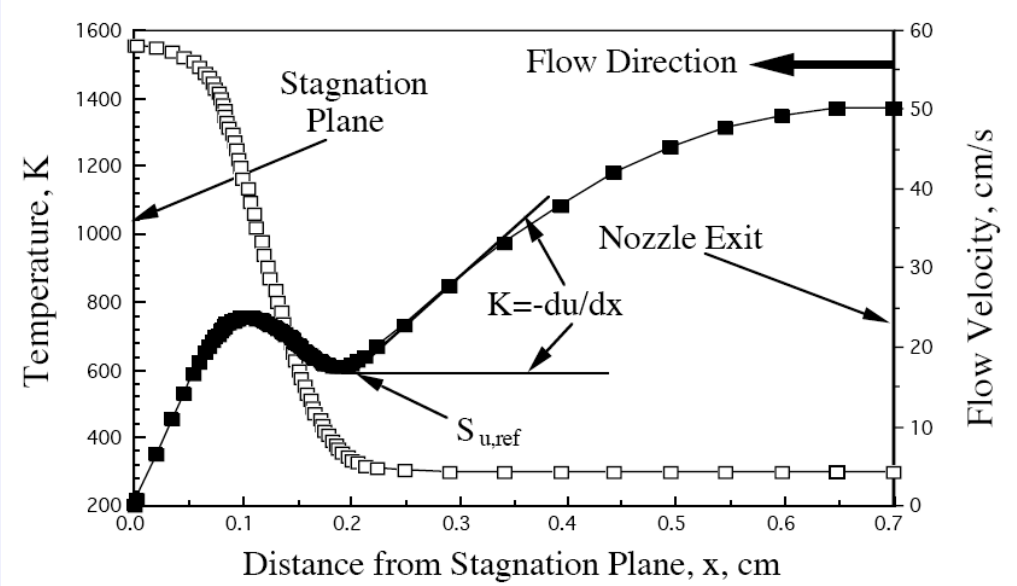


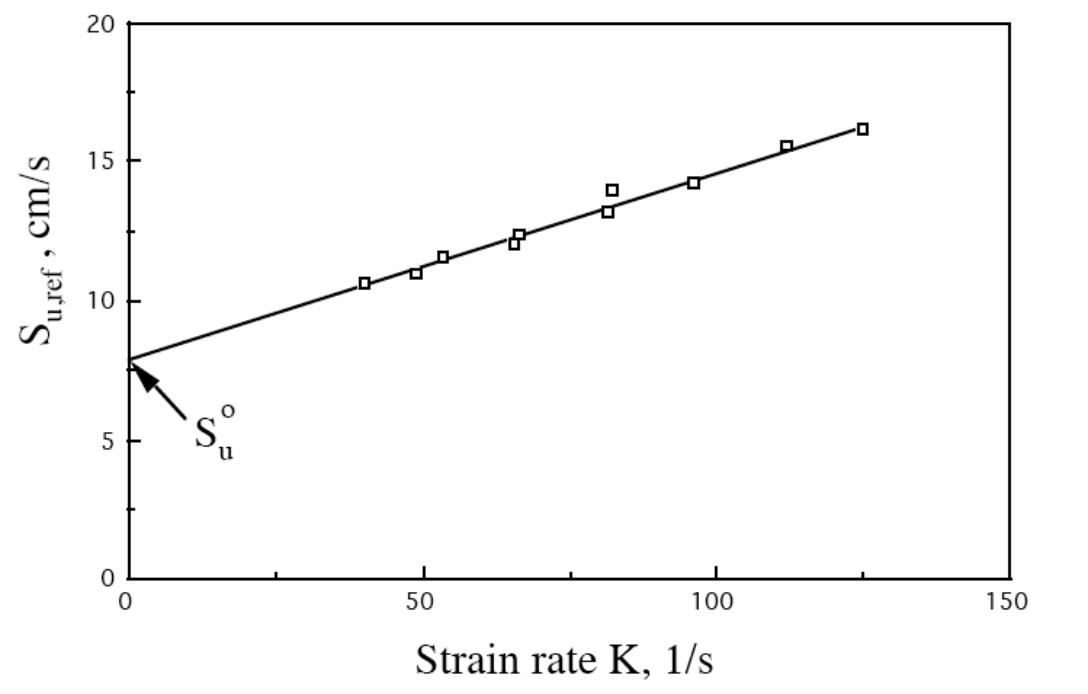
- **The sensitivity analysis includes**
  - **Kinetics**
  - **Molecular transport (binary diffusion coefficients)**
- **PREMIX code modified to account for sensitivity analysis on diffusion**
- **Opposed jet code can treat strain rate or ignition temperature as dependent variable and sensitivity analysis for the extinction strain rate can be performed**
- **Logarithmic sensitivity coefficients: $\partial(\ln Y)/\partial(\ln X)$**
  - **Y: laminar flame speed / extinction strain rate / ignition temperature**
  - **X: A-factor / $D_{i\text{-}N2}$**

Propagation and Extinction of n-Paraffin/Air and JP-8/air Flames

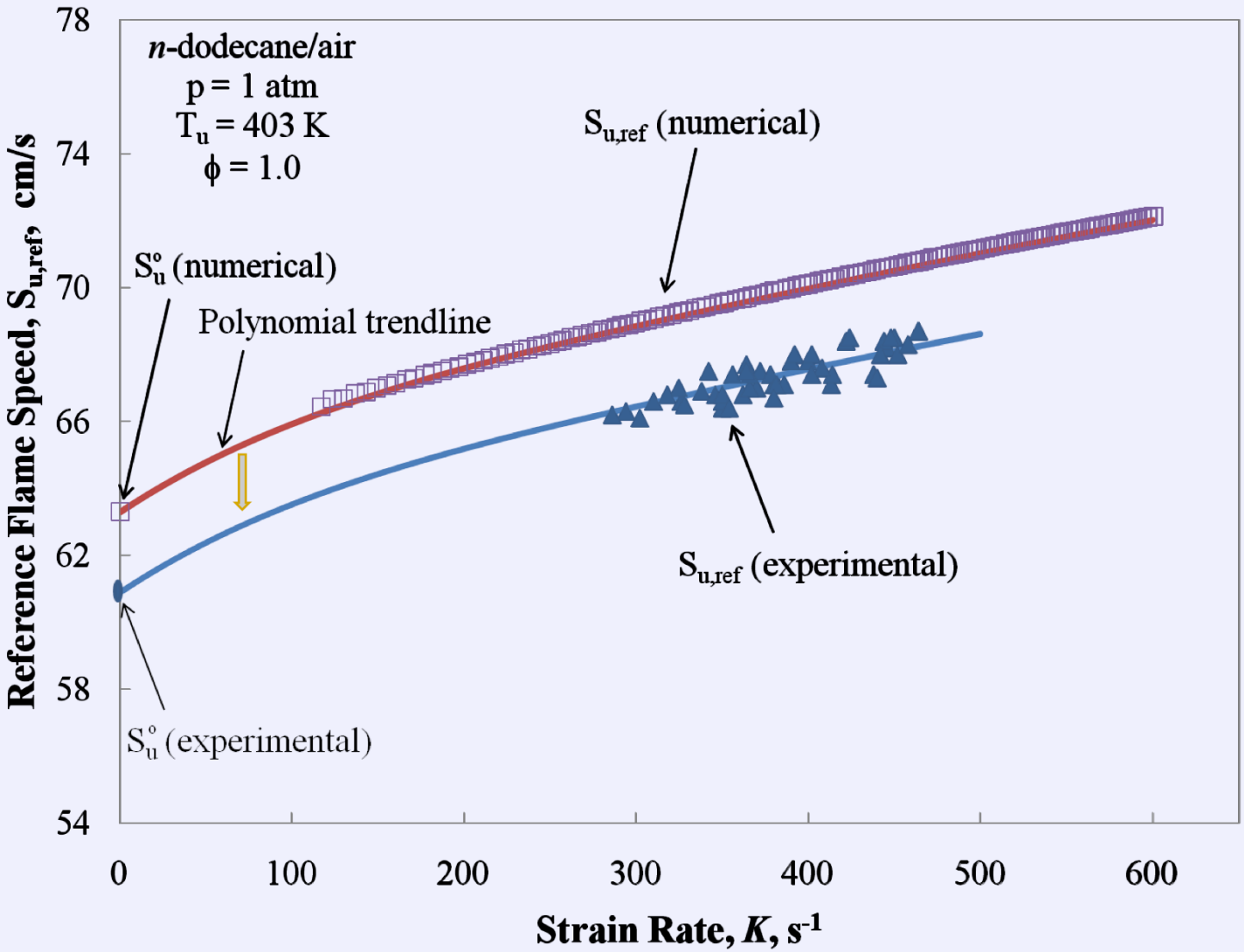
Propagation of Stagnation-Type Flames







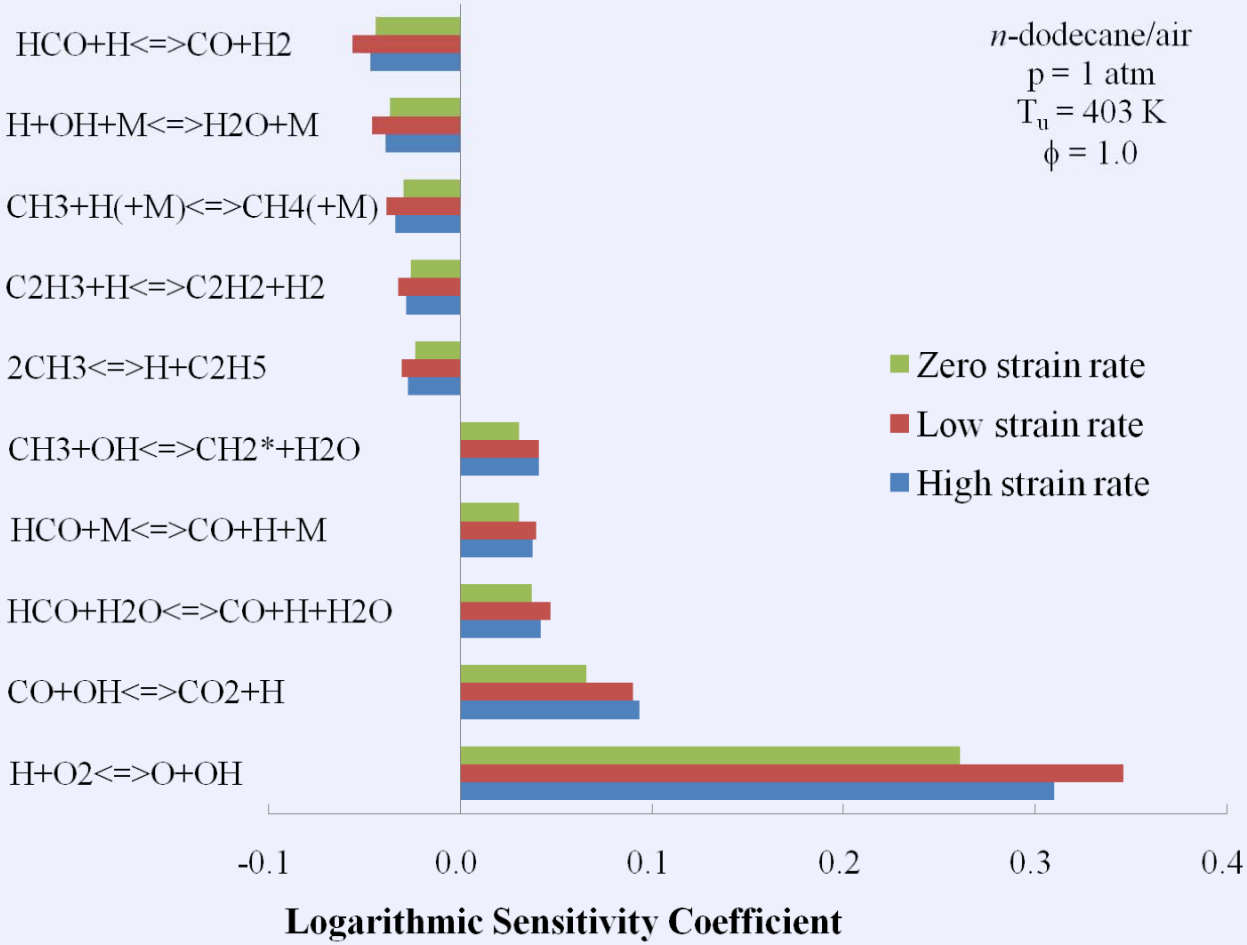
A New Computationally-Assisted Extrapolation* (1)

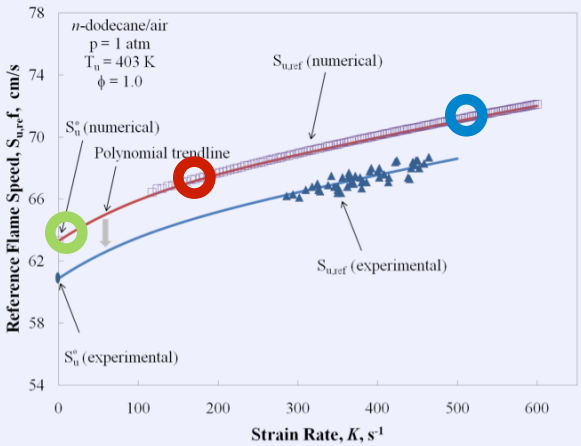


***First introduced for DME/air flames in:**

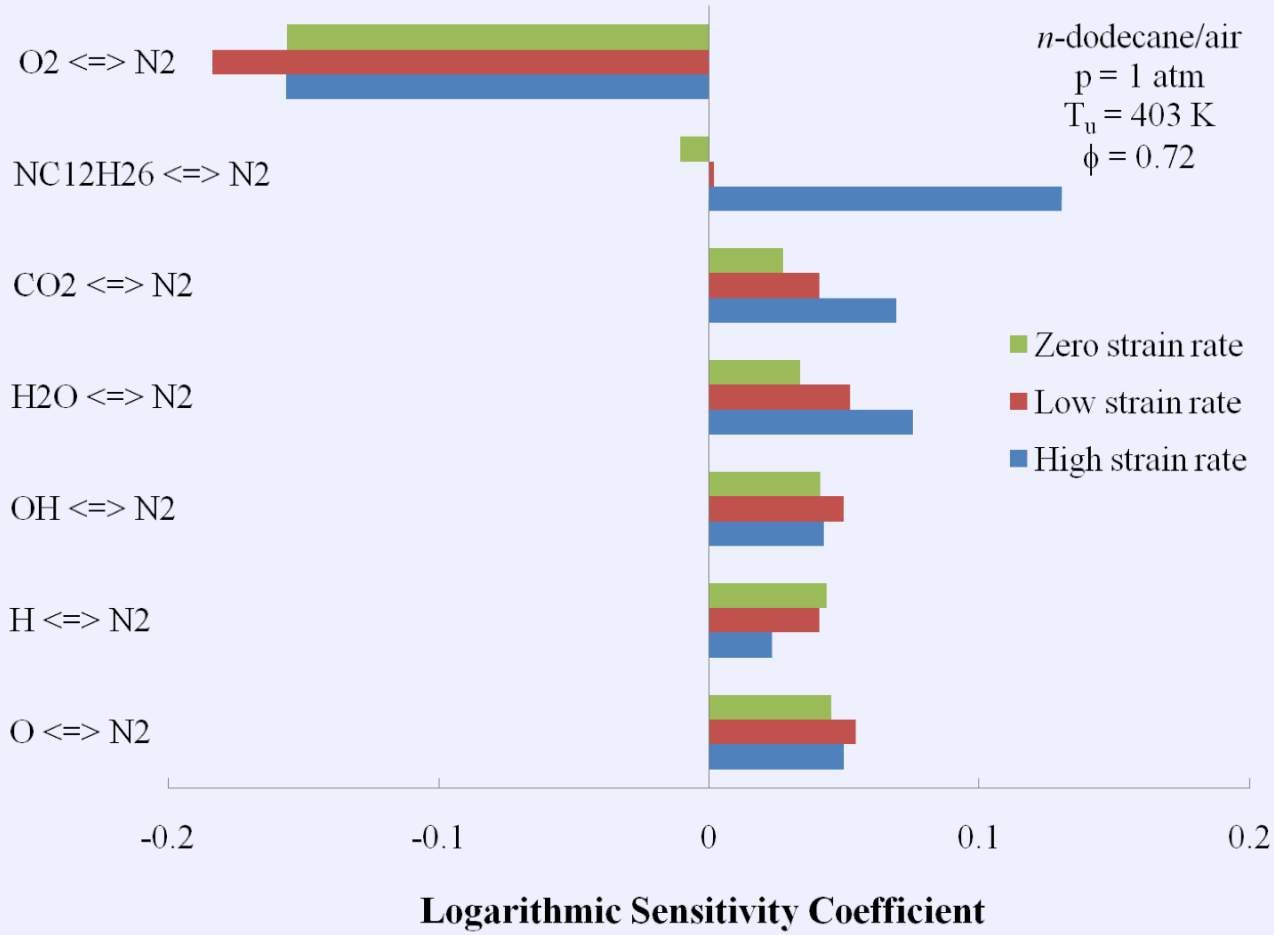
Y.L. Wang, A.T. Holley, C. Ji, F.N. Egolfopoulos, T.T. Tsotsis, H.J. Curran, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

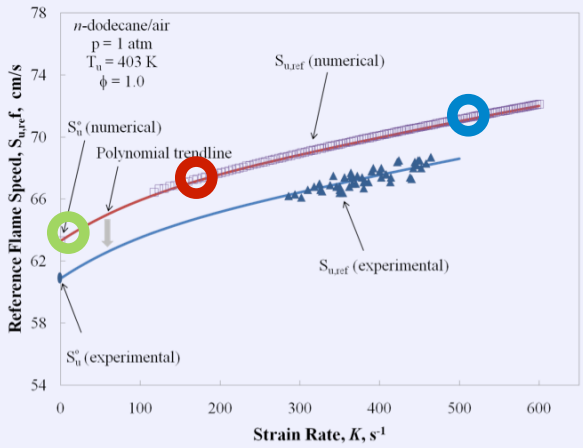
A New Computationally-Assisted Extrapolation (2)



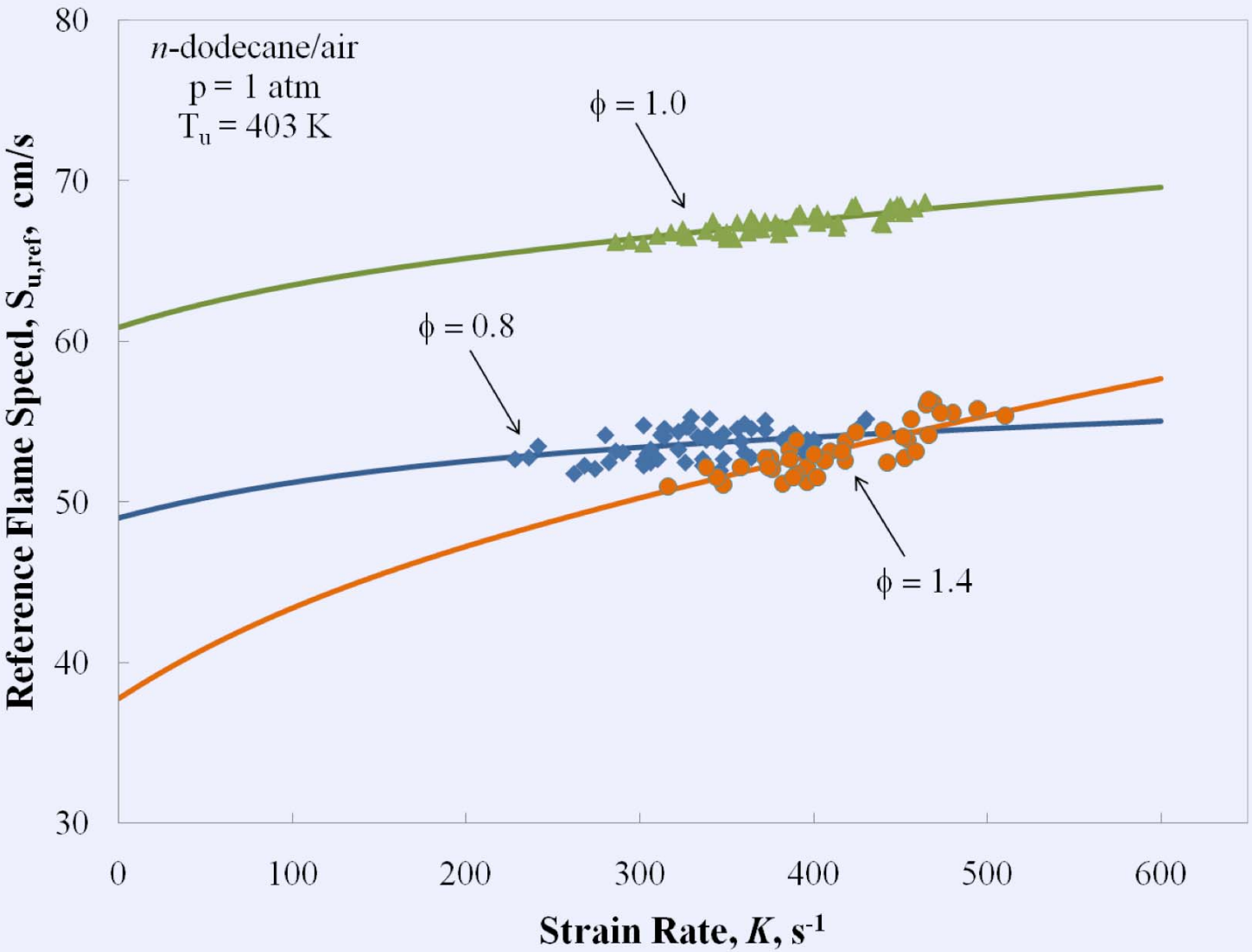


A New Computationally-Assisted Extrapolation (3)



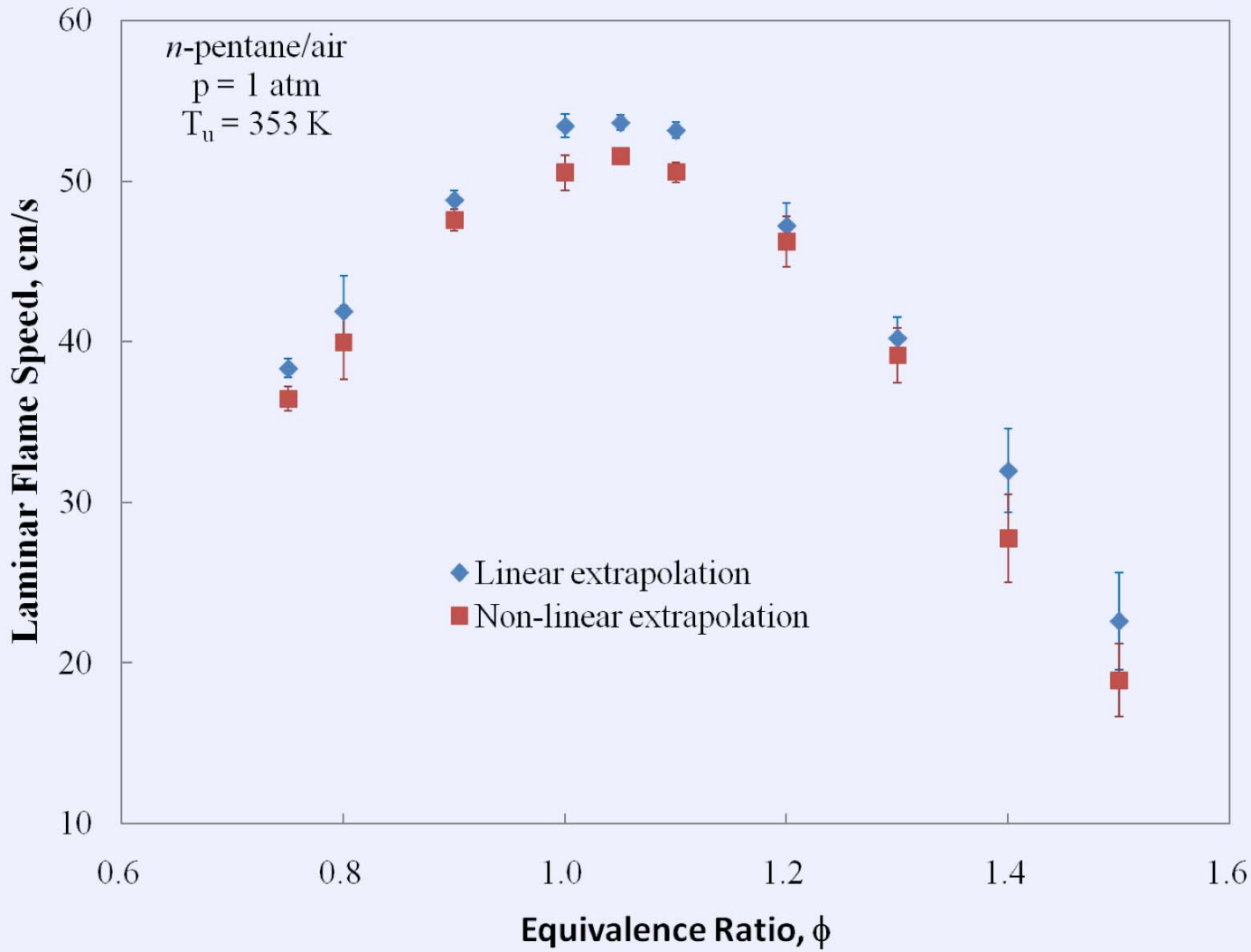


A New Computationally-Assisted Extrapolation[1] (4)



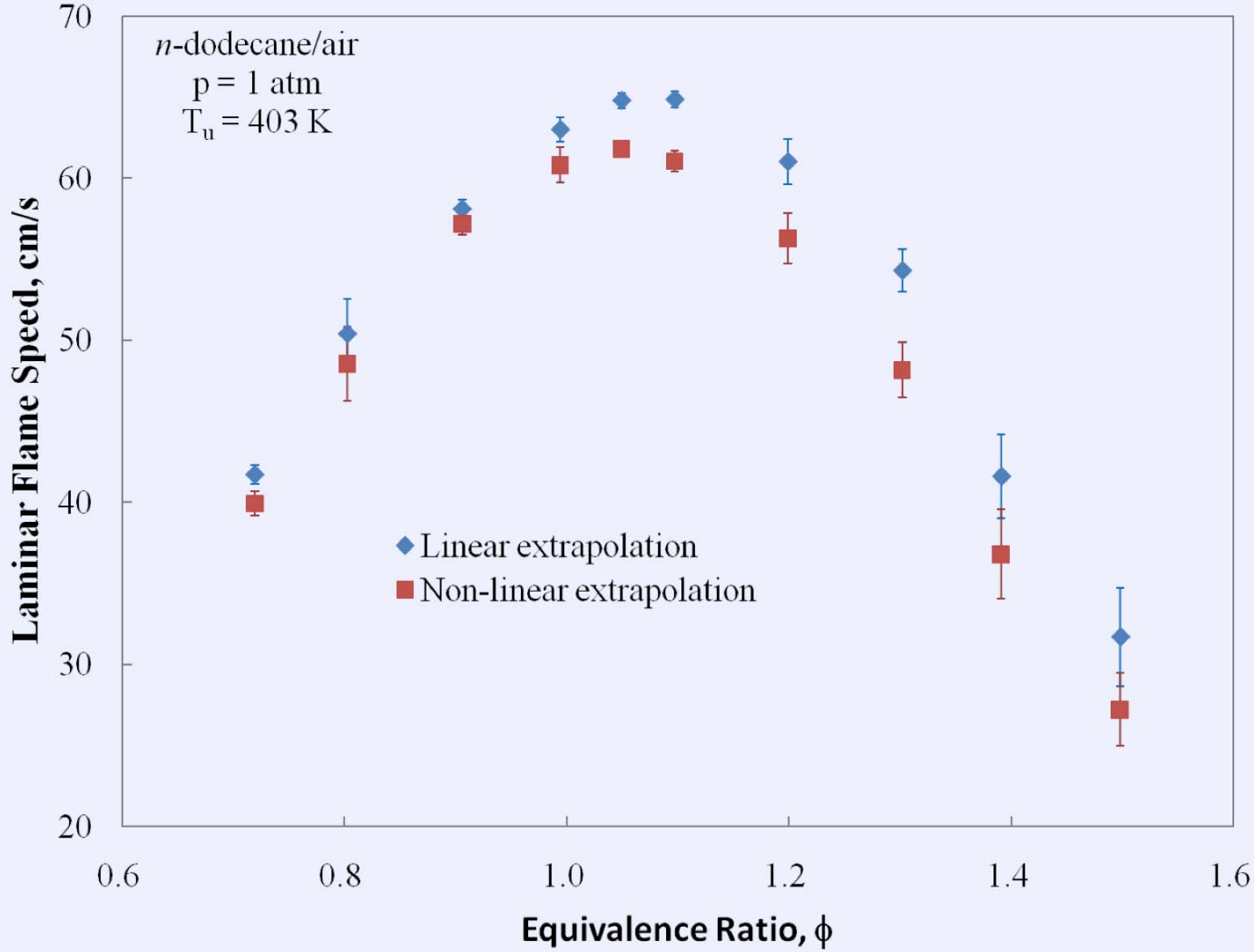
[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Effect of Non-Linear Extrapolations for n-Pentane[1]



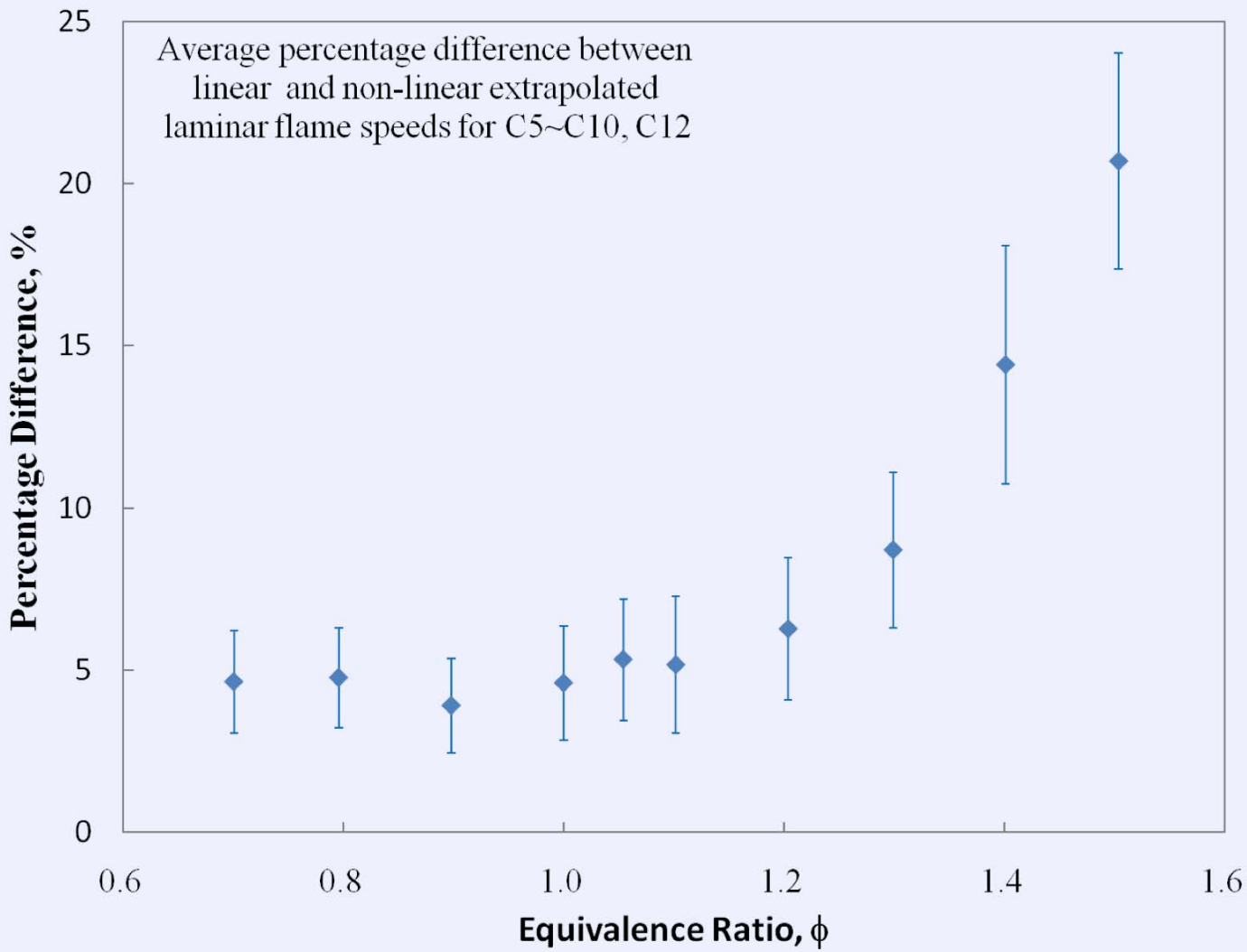
[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Effect of Non-Linear Extrapolations for n-Dodecane[1]



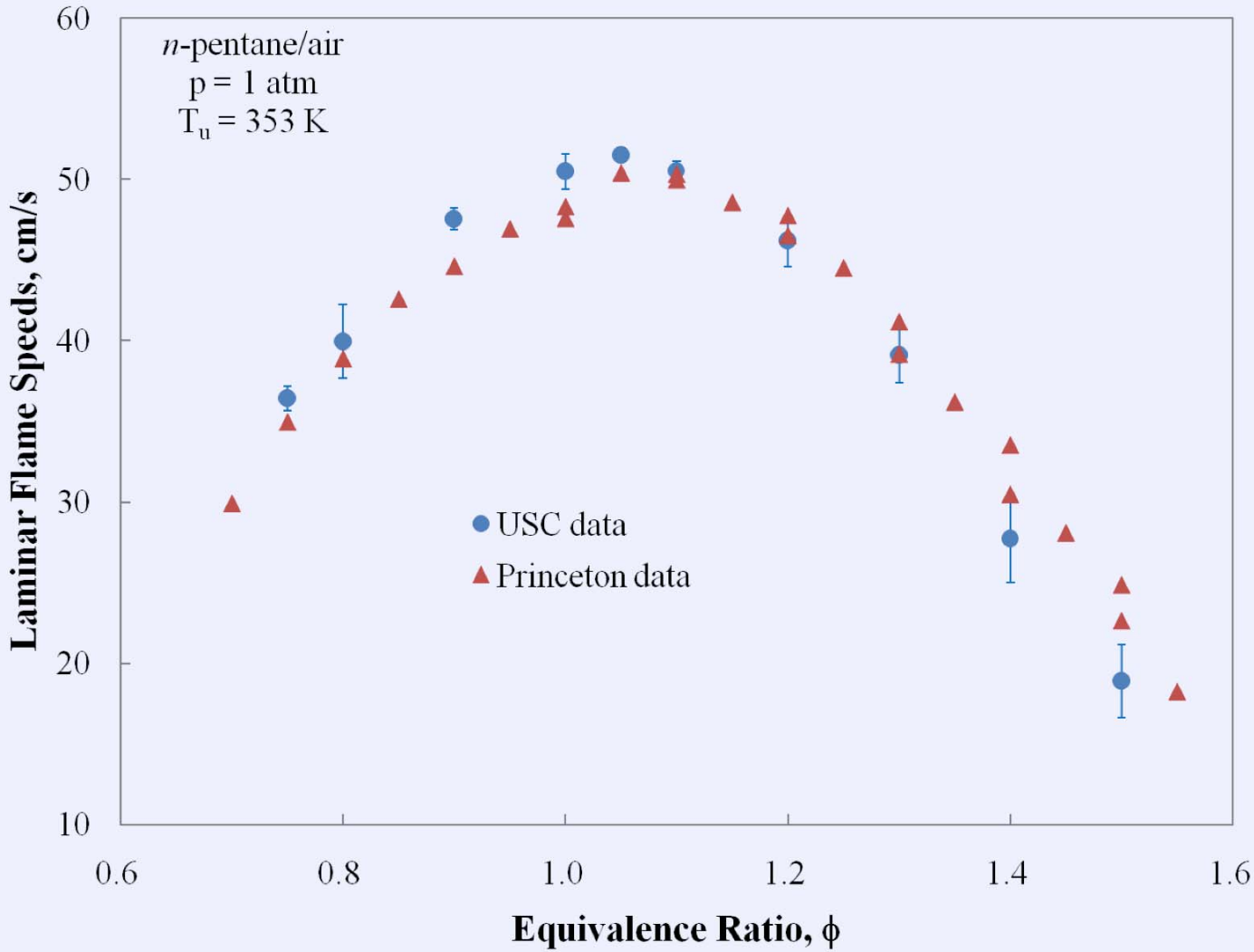
[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Effect of Non-Linear Extrapolation for All Fuels[1]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

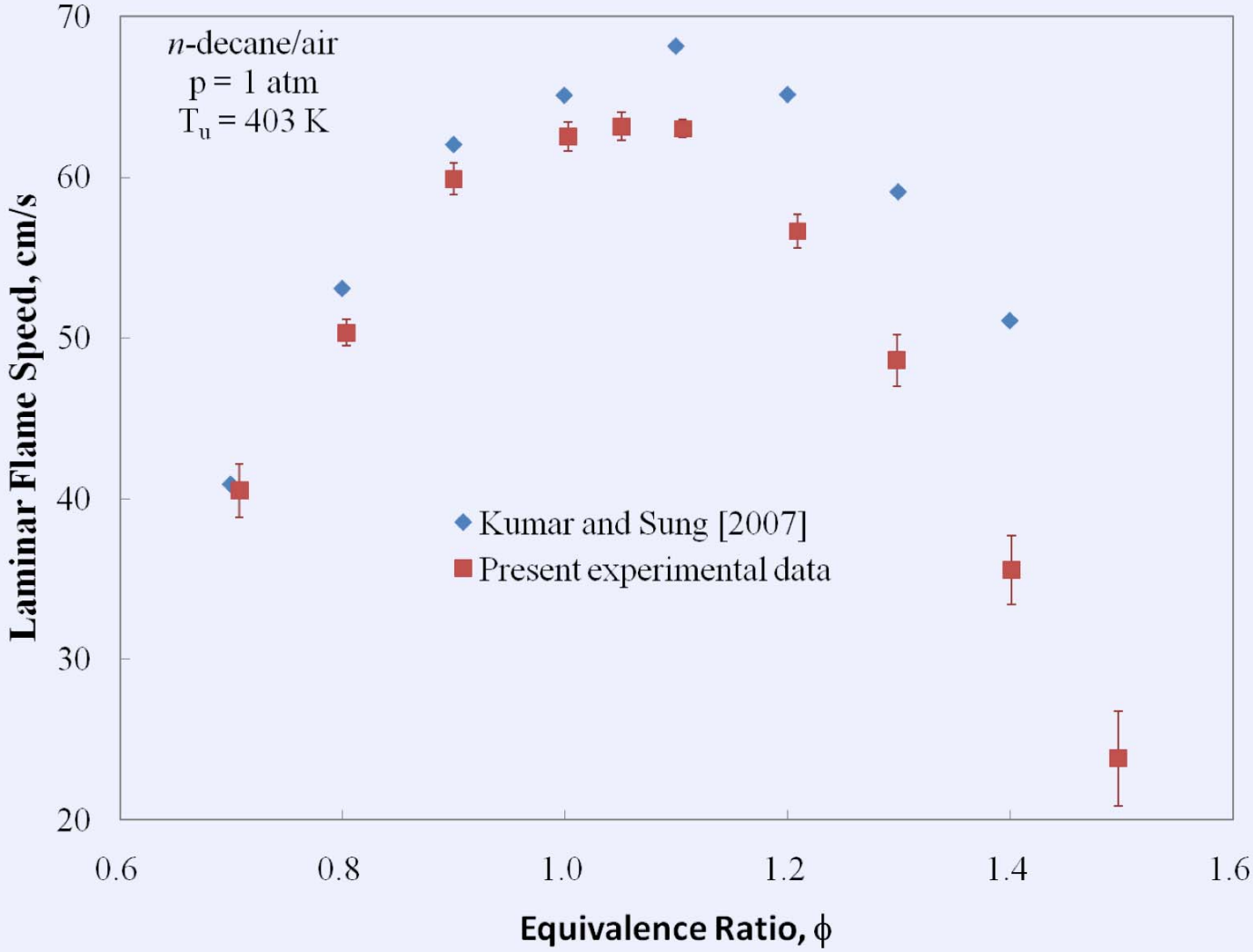
Comparison with Princeton n-Pentane Data[1,2]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

[2]A. Kelley, C.K. Law, and coworkers, unpublished data (2008)

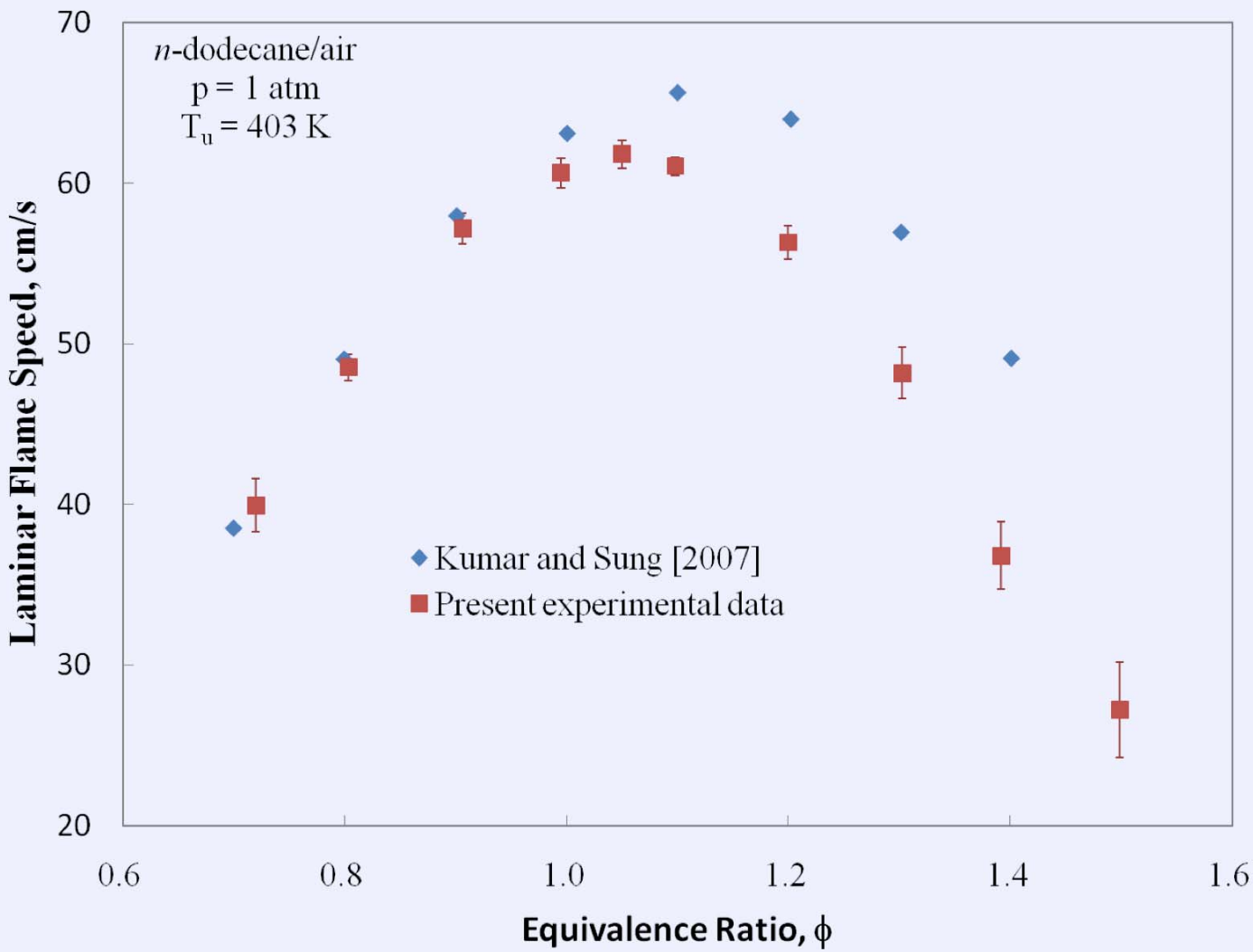
Comparison with Case Western n-Decane Data[1,3]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

[3]K. Kumar, C.J. Sung, *Combustion and Flame* 151: 2095-224 (2007)

Comparison with Case Western n-Dodecane Data[1,3]



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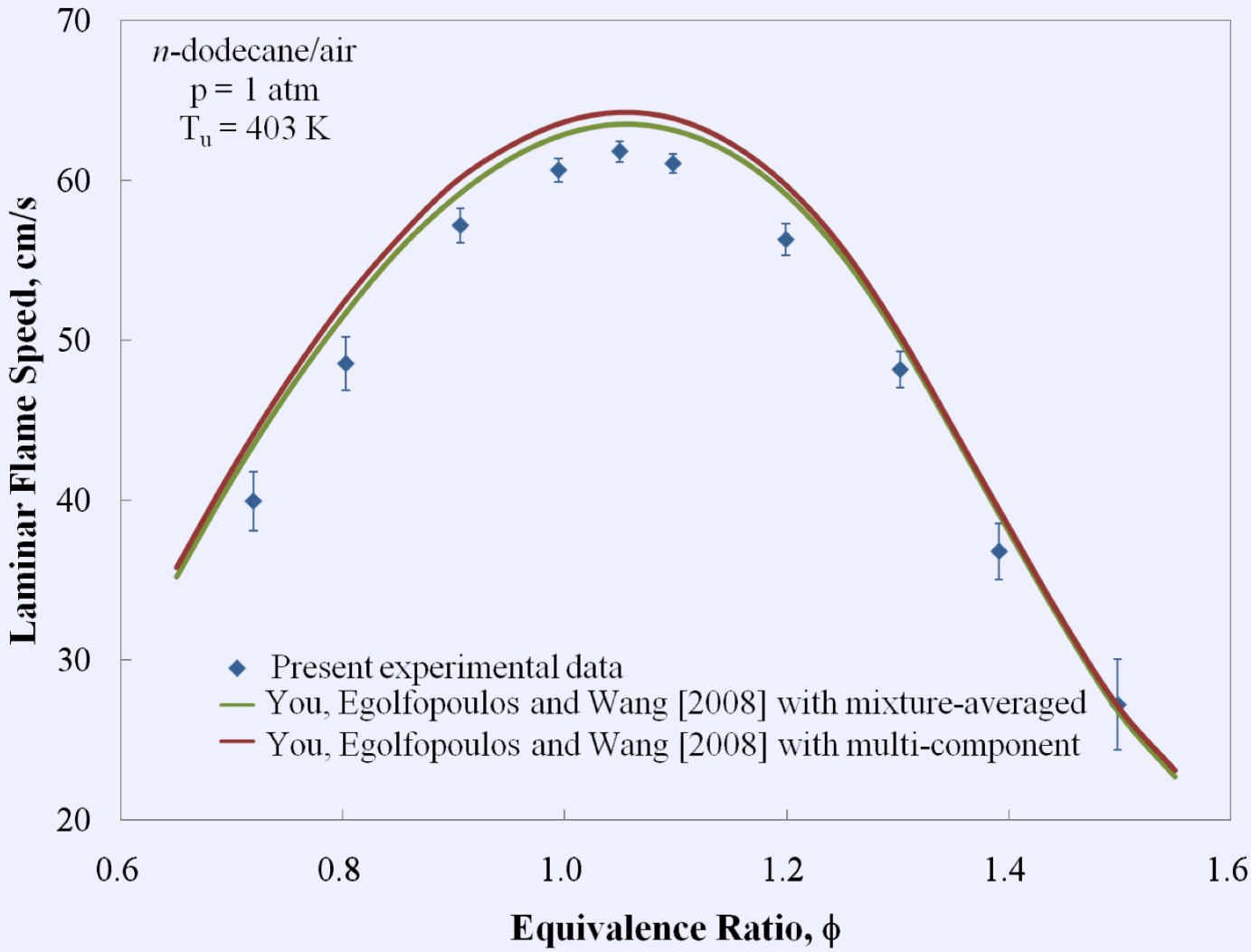
[3]K. Kumar, C.J. Sung, *Combustion and Flame* 151: 2095-224 (2007)

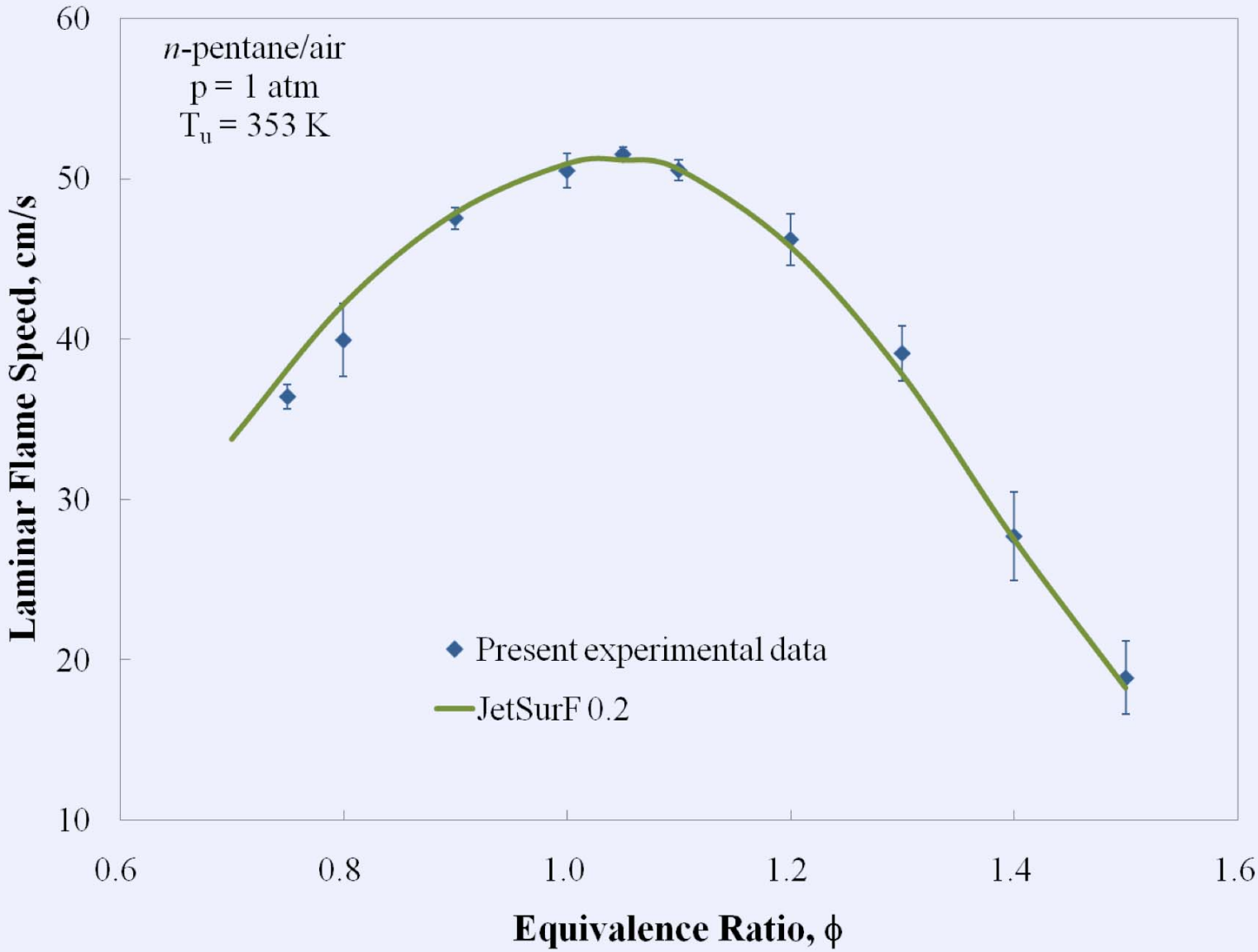
Effect of Transport Model on Laminar Flame Speeds[1,4]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

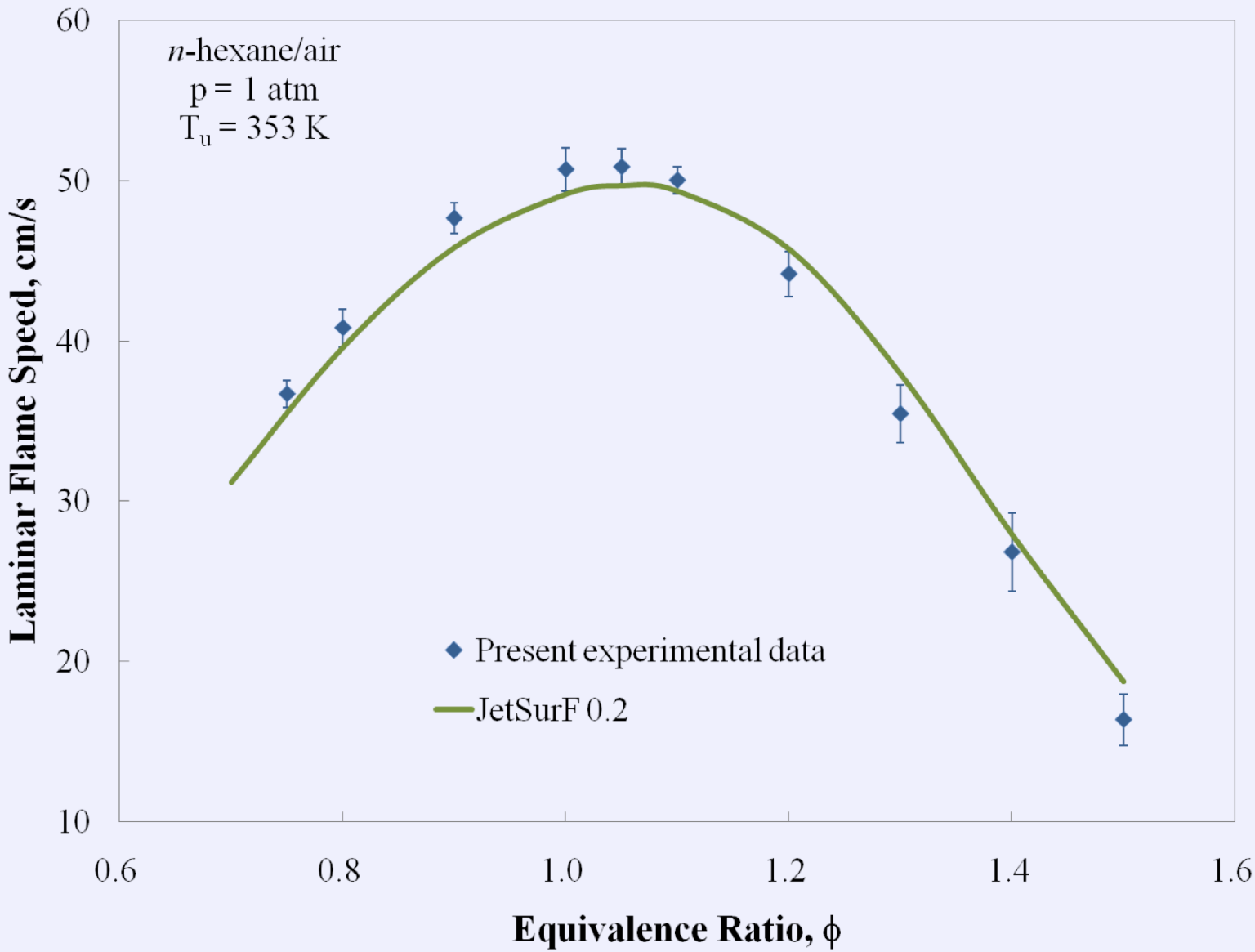
[4]X.Q. You, F.N. Egolfopoulos, H. Wang, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

Laminar Flame Speeds of n-Pentane/Air Flames[1]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Laminar Flame Speeds of n-Hexane/Air Flames[1]



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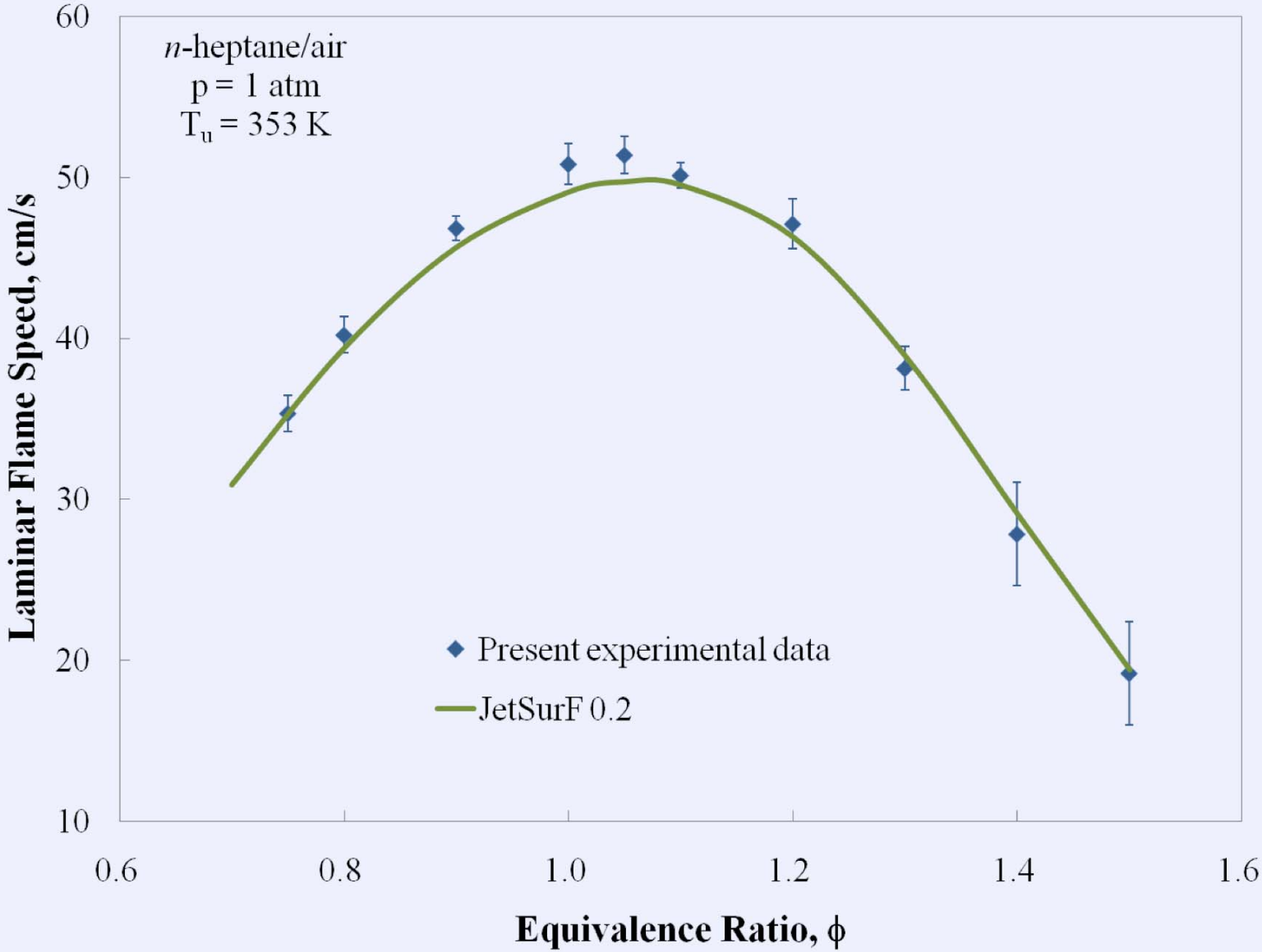
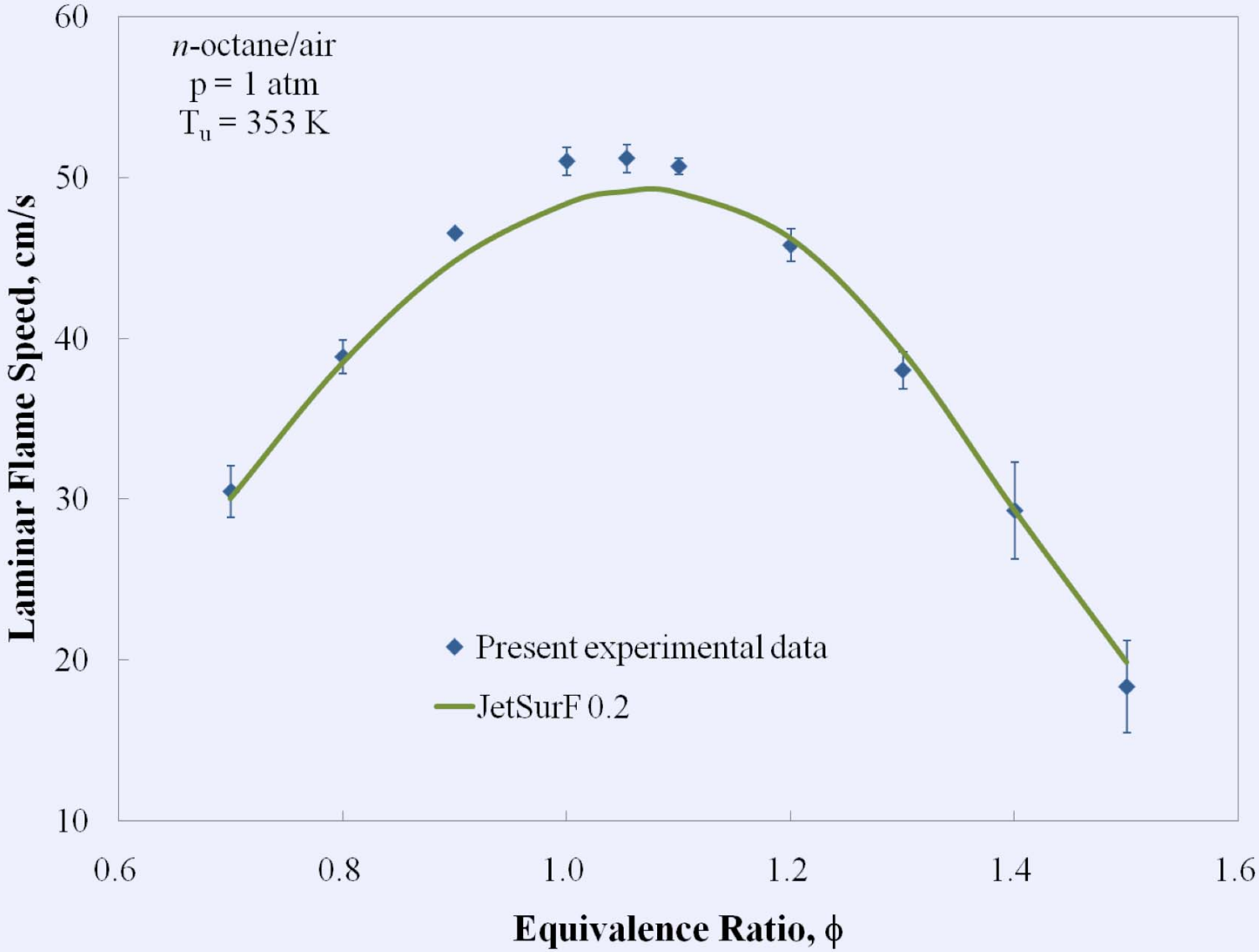
Laminar Flame Speeds of n-Heptane/Air Flames[1]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Laminar Flame Speeds of n-Octane/Air Flames[1]



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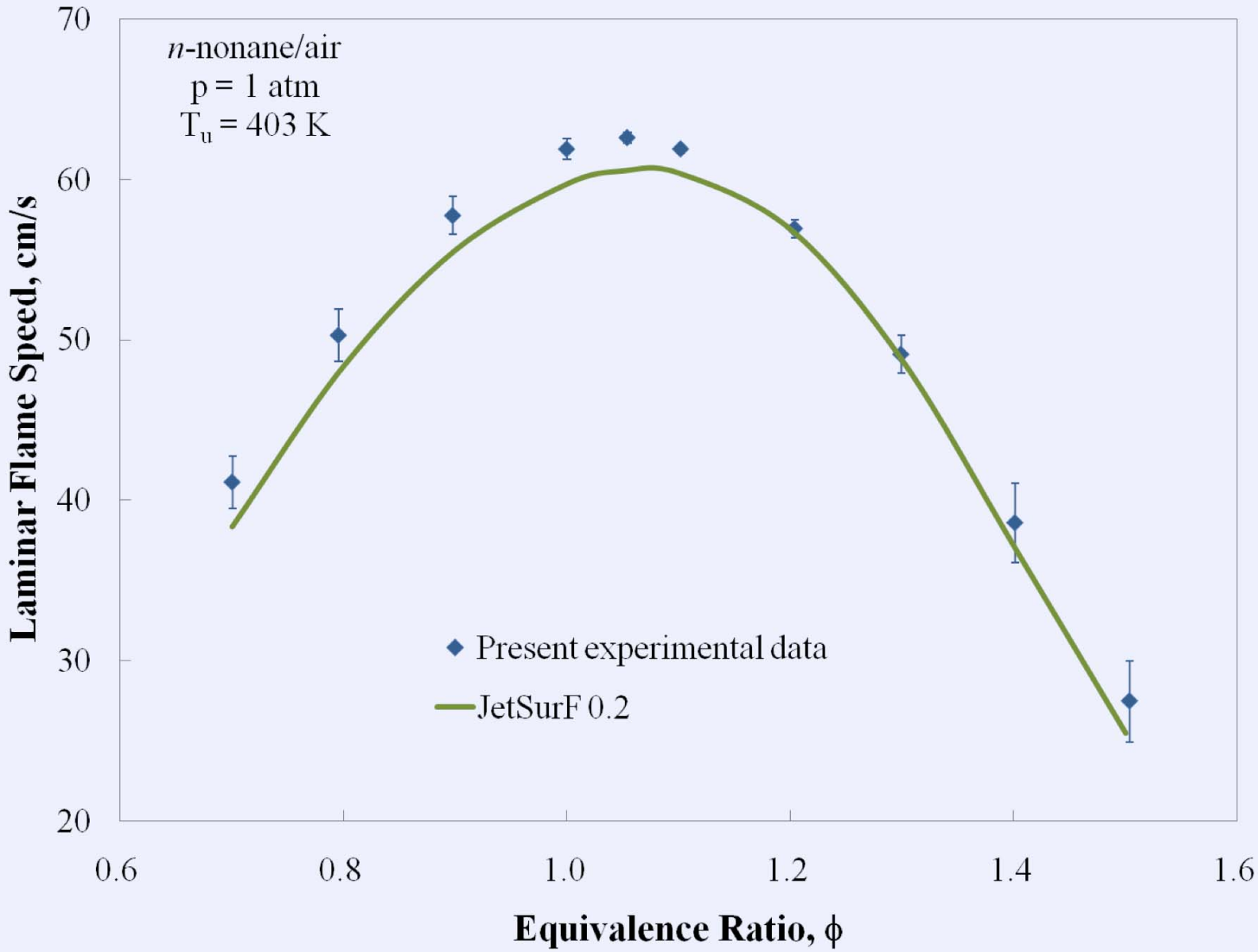
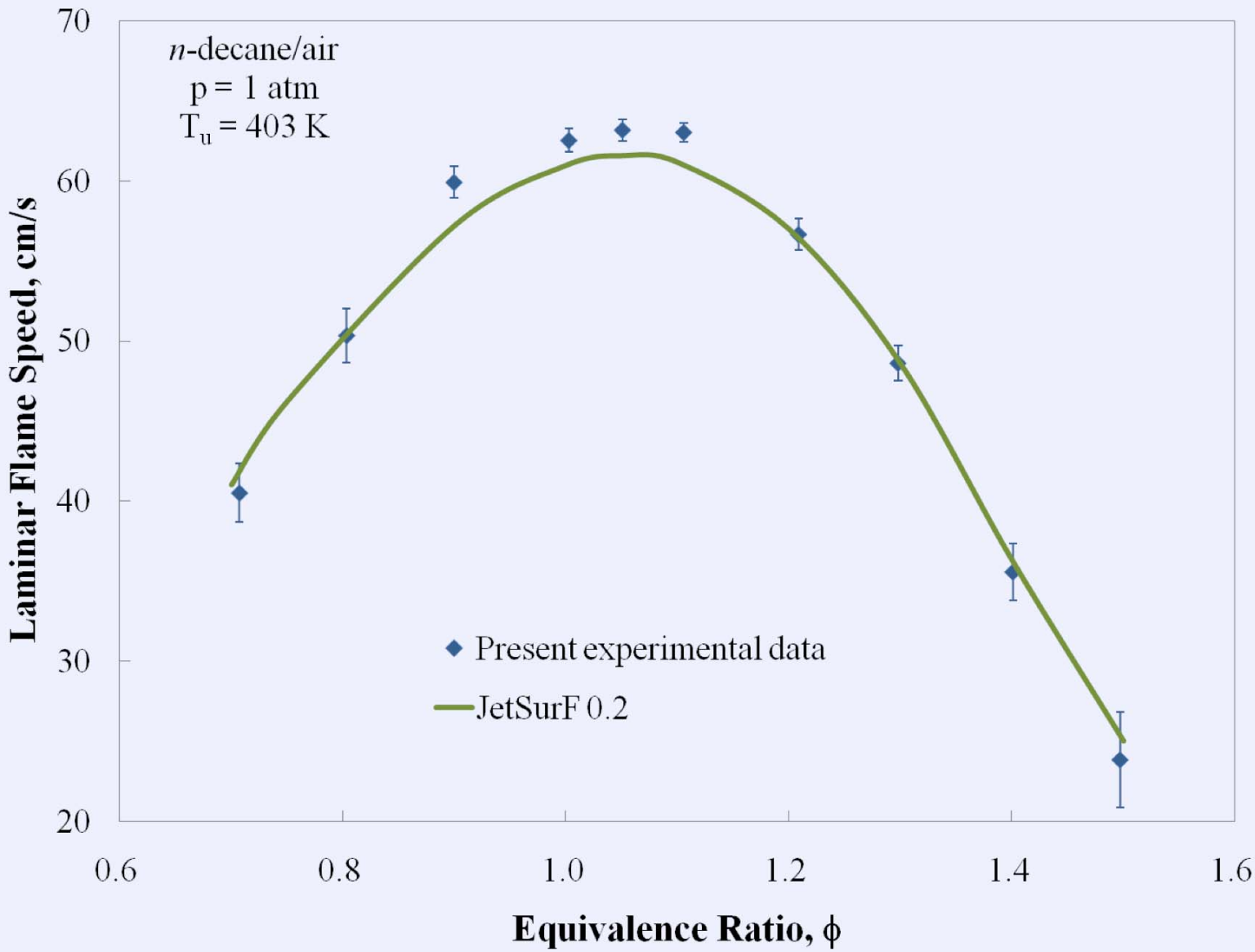
Laminar Flame Speeds of n-Nonane/Air Flames[1]



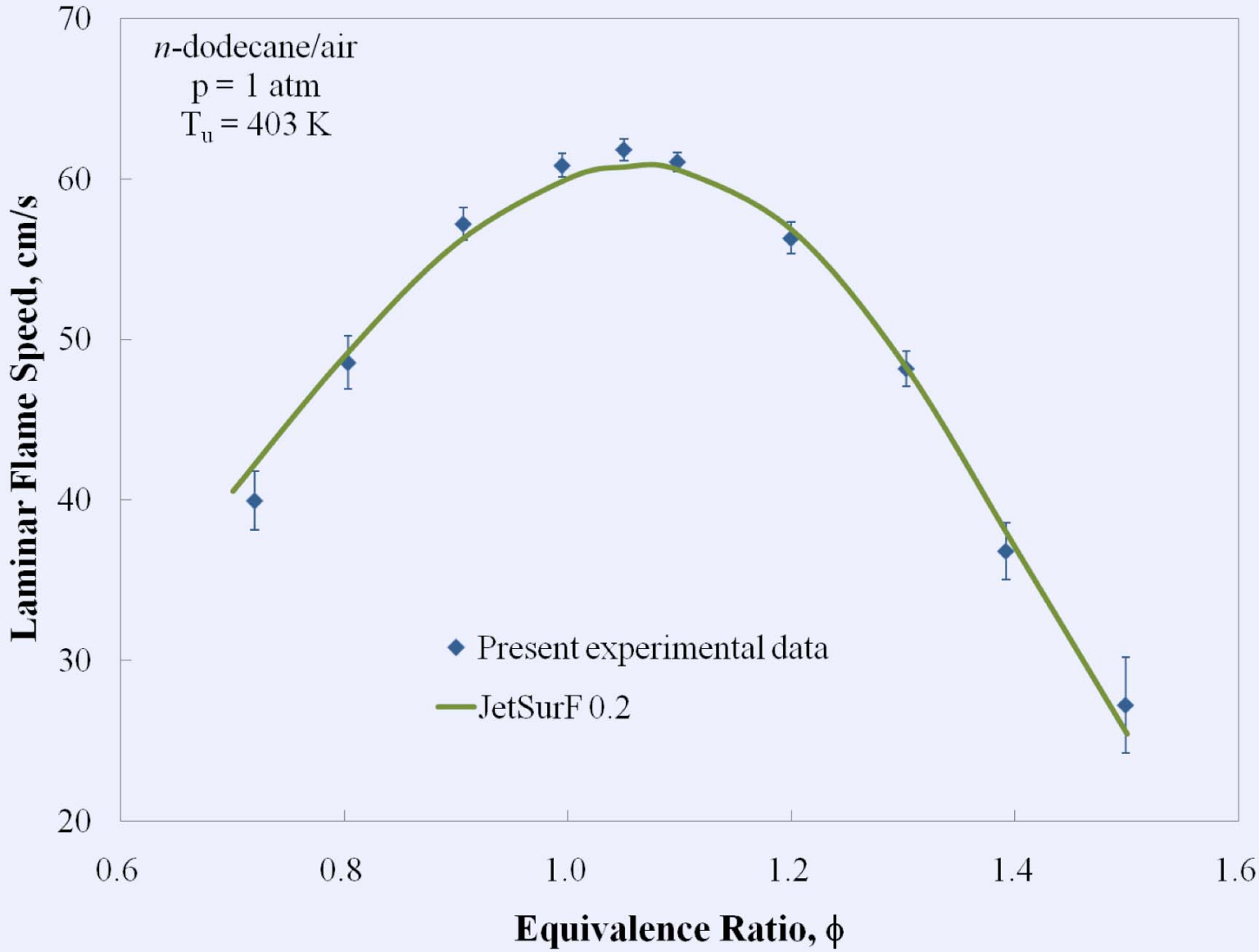
[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Laminar Flame Speeds of n-Decane/Air Flames[1]



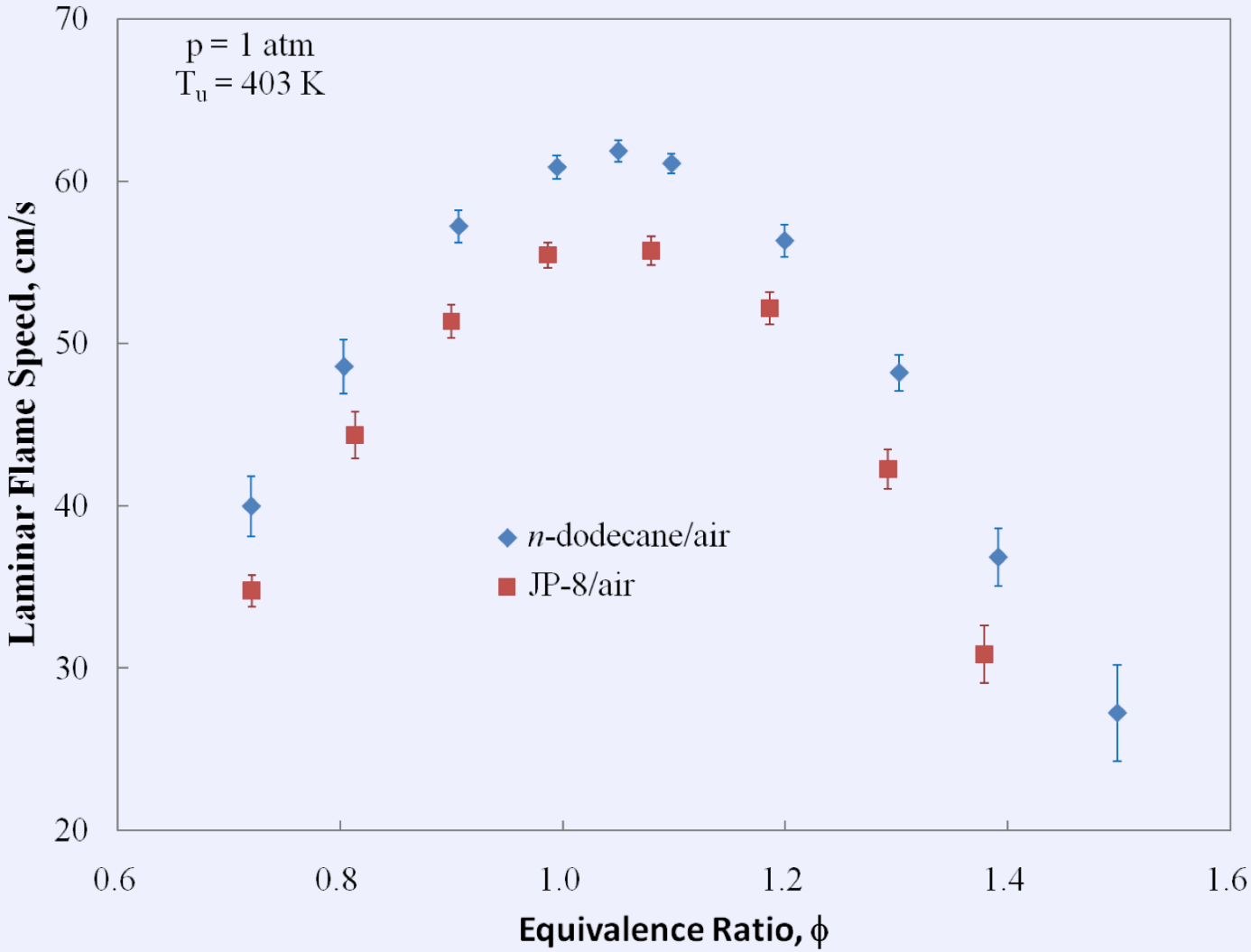
[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Laminar Flame Speeds of n-Dodecane/Air Flames[1]



[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Flame Propagation: n-Dodecane vs. JP-8[1]



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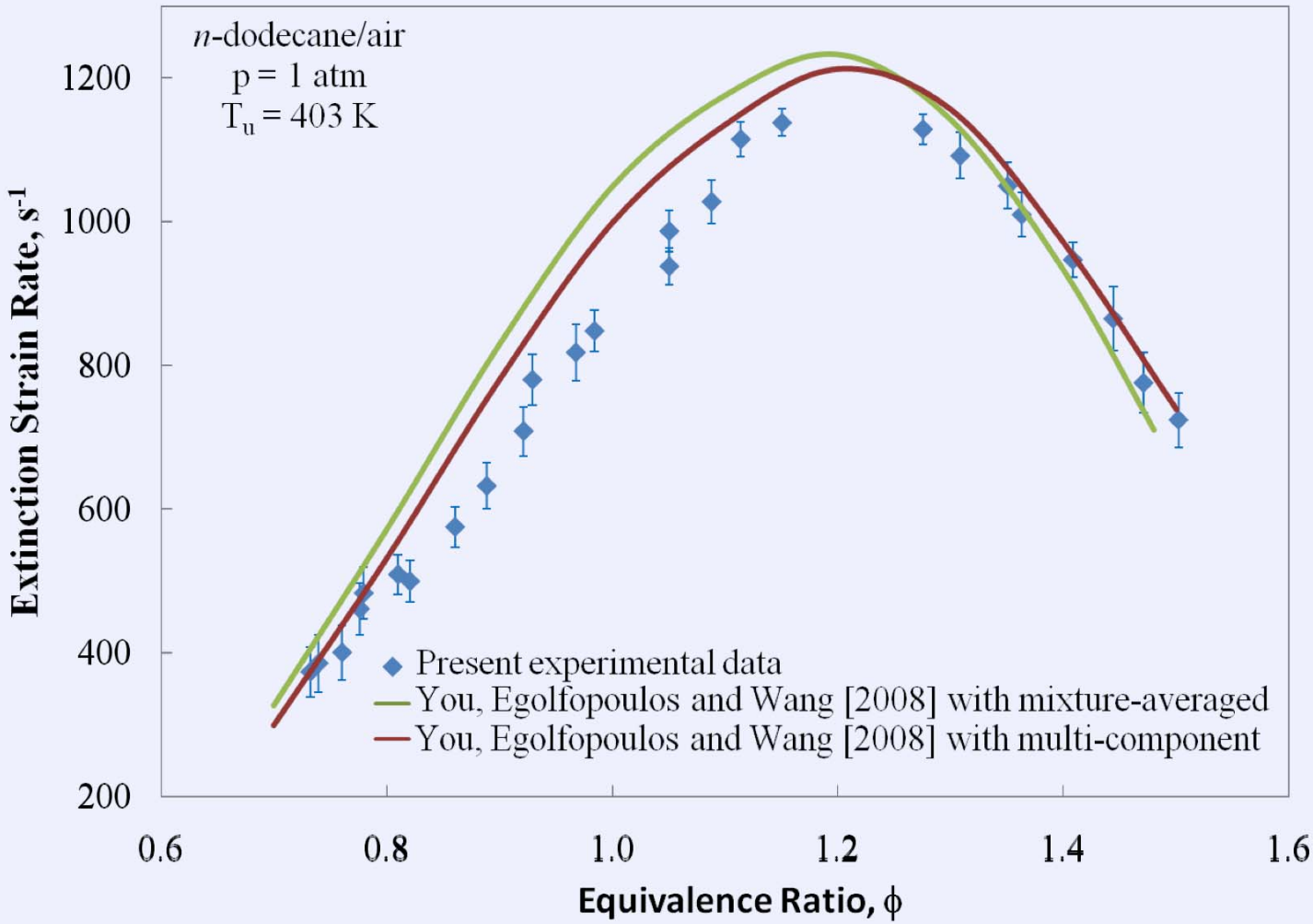
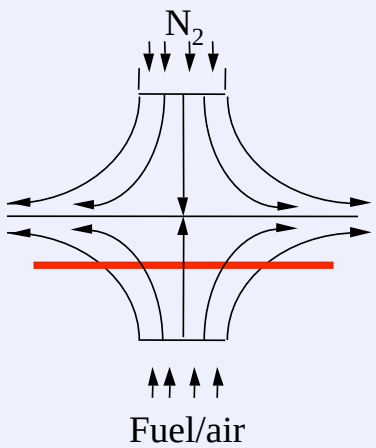
Effect of Transport Model on Extinction Response[1,4]





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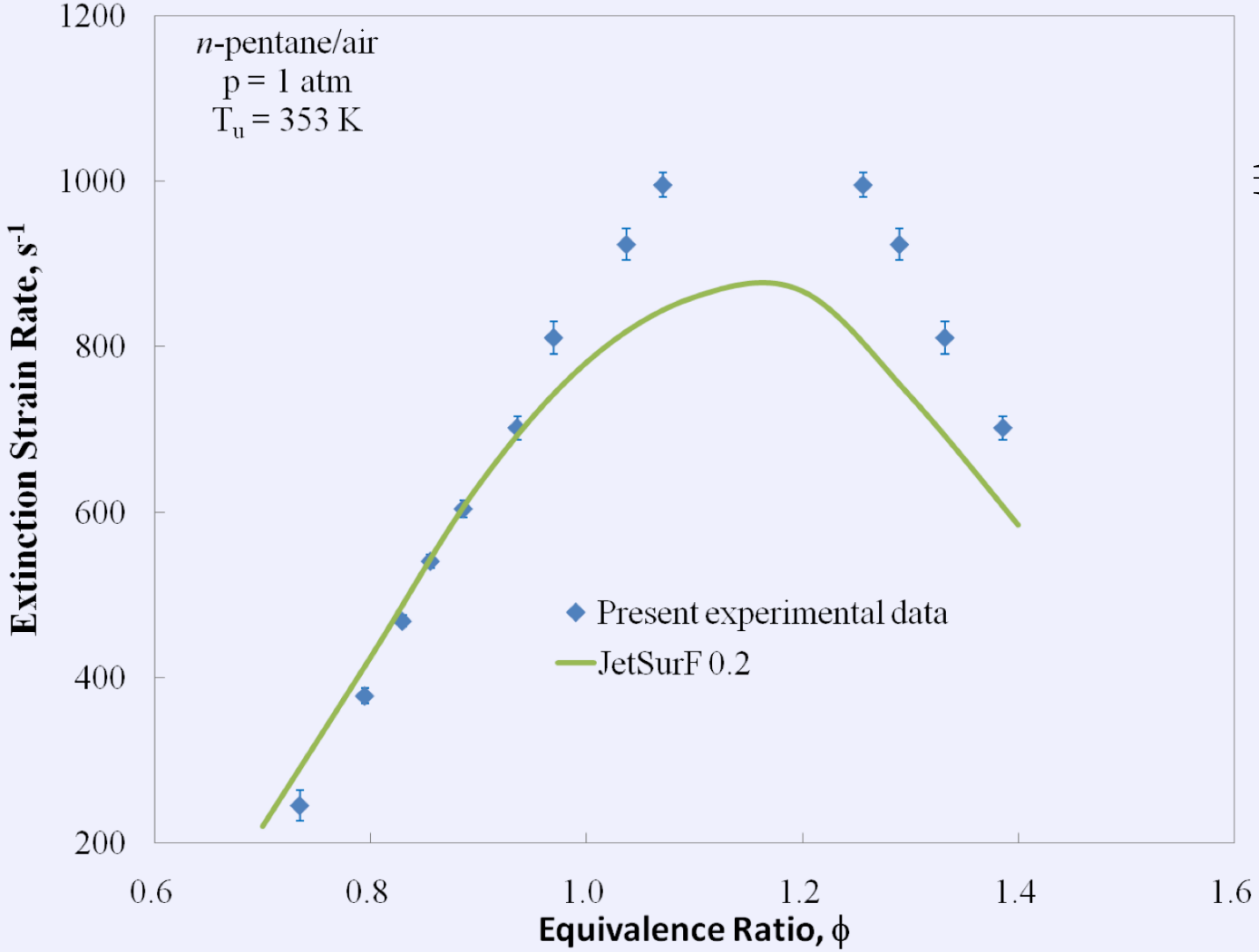
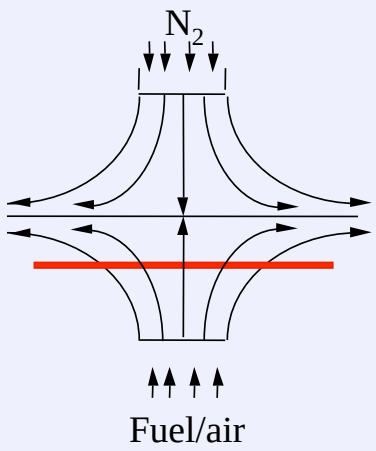
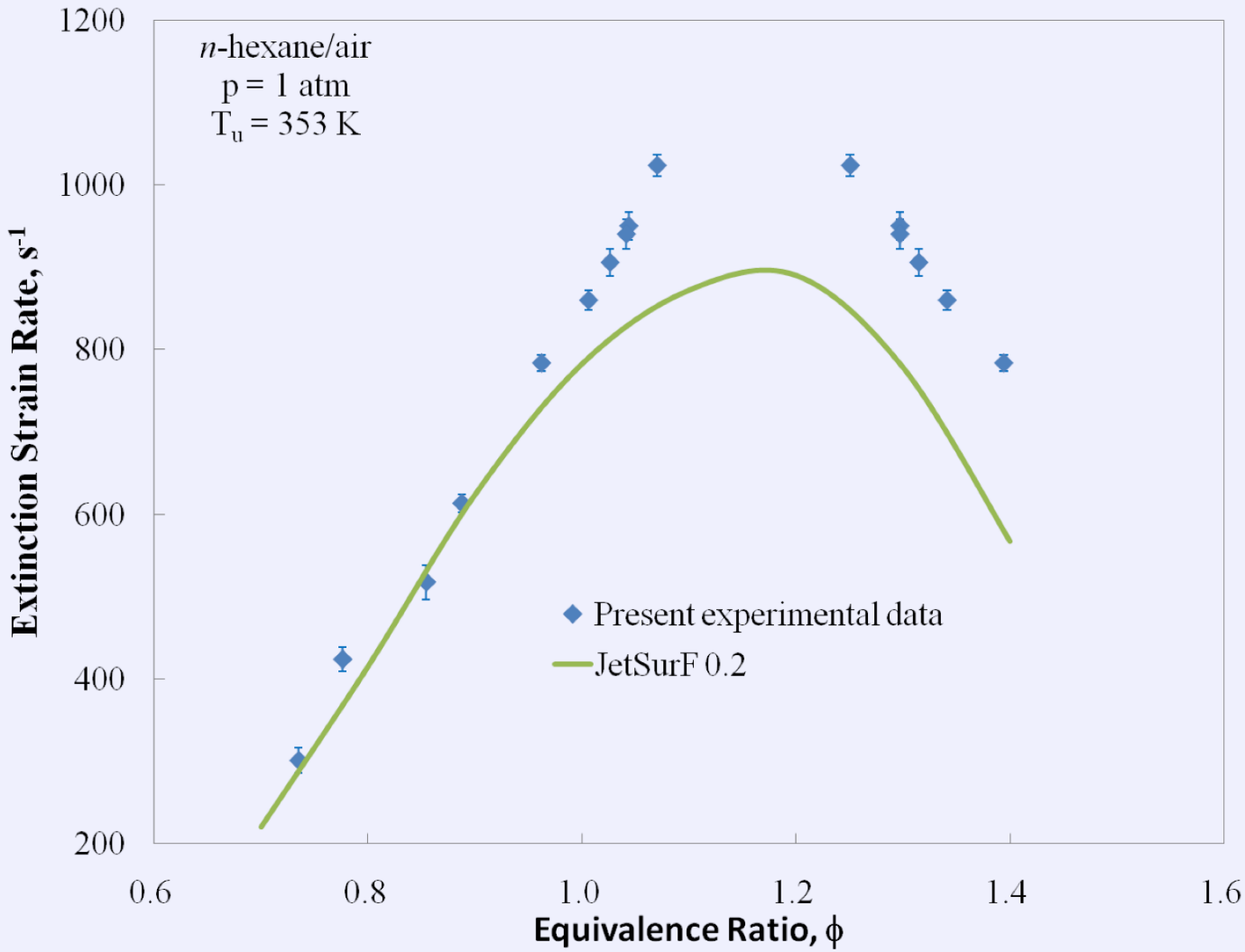
Extinction Strain Rates of n-Pentane/Air Flames[1]

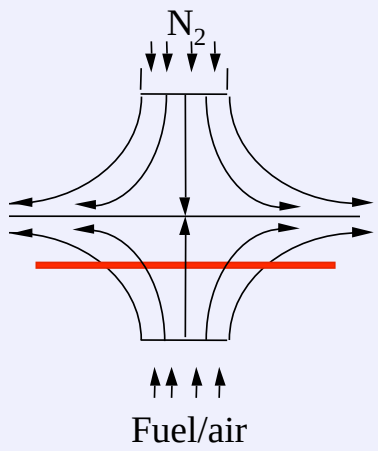




[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Extinction Strain Rates of n-Hexane/Air Flames[1]





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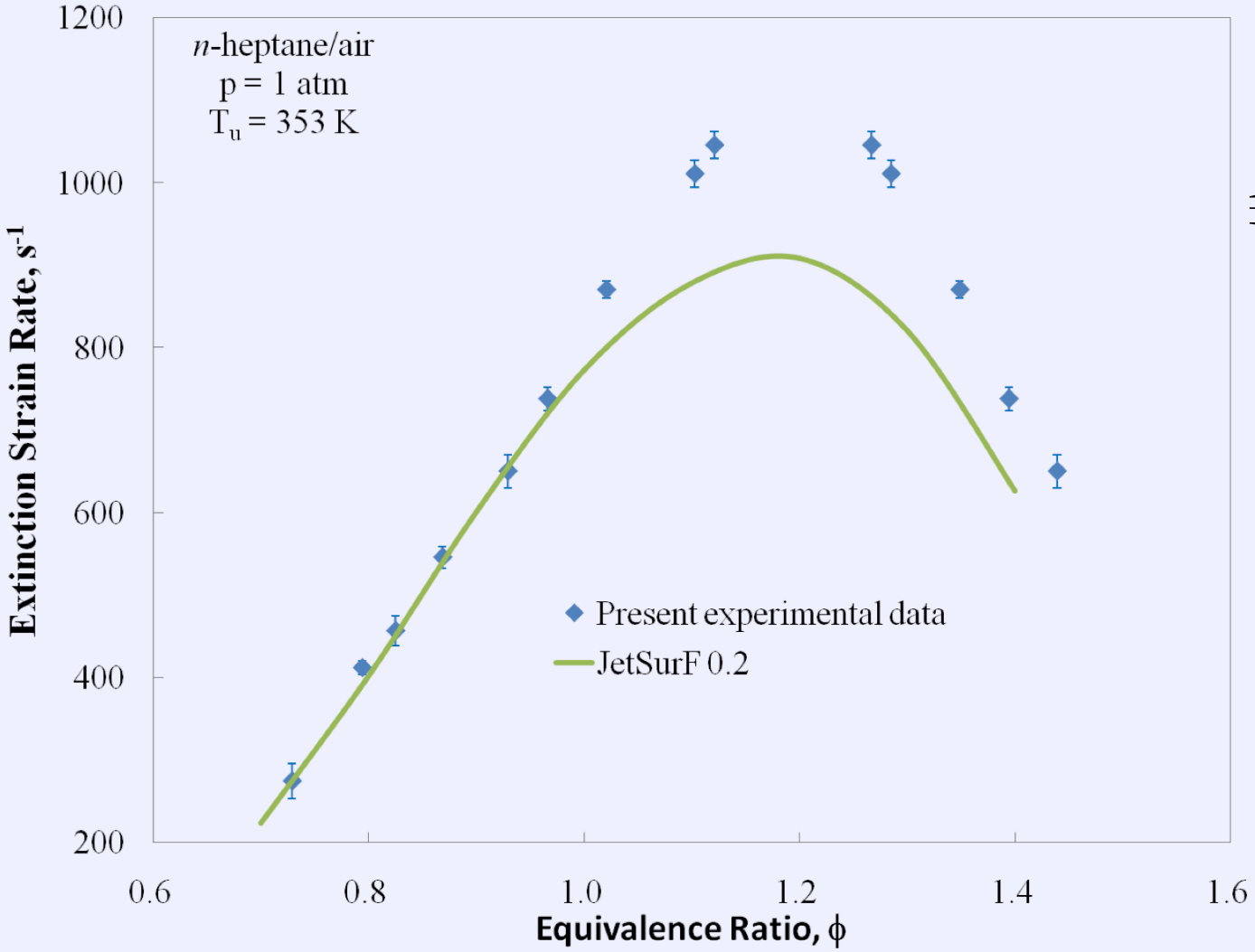
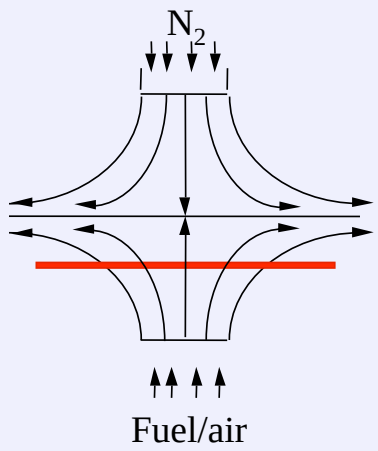
Extinction Strain Rates of n-Heptane/Air Flames[1]





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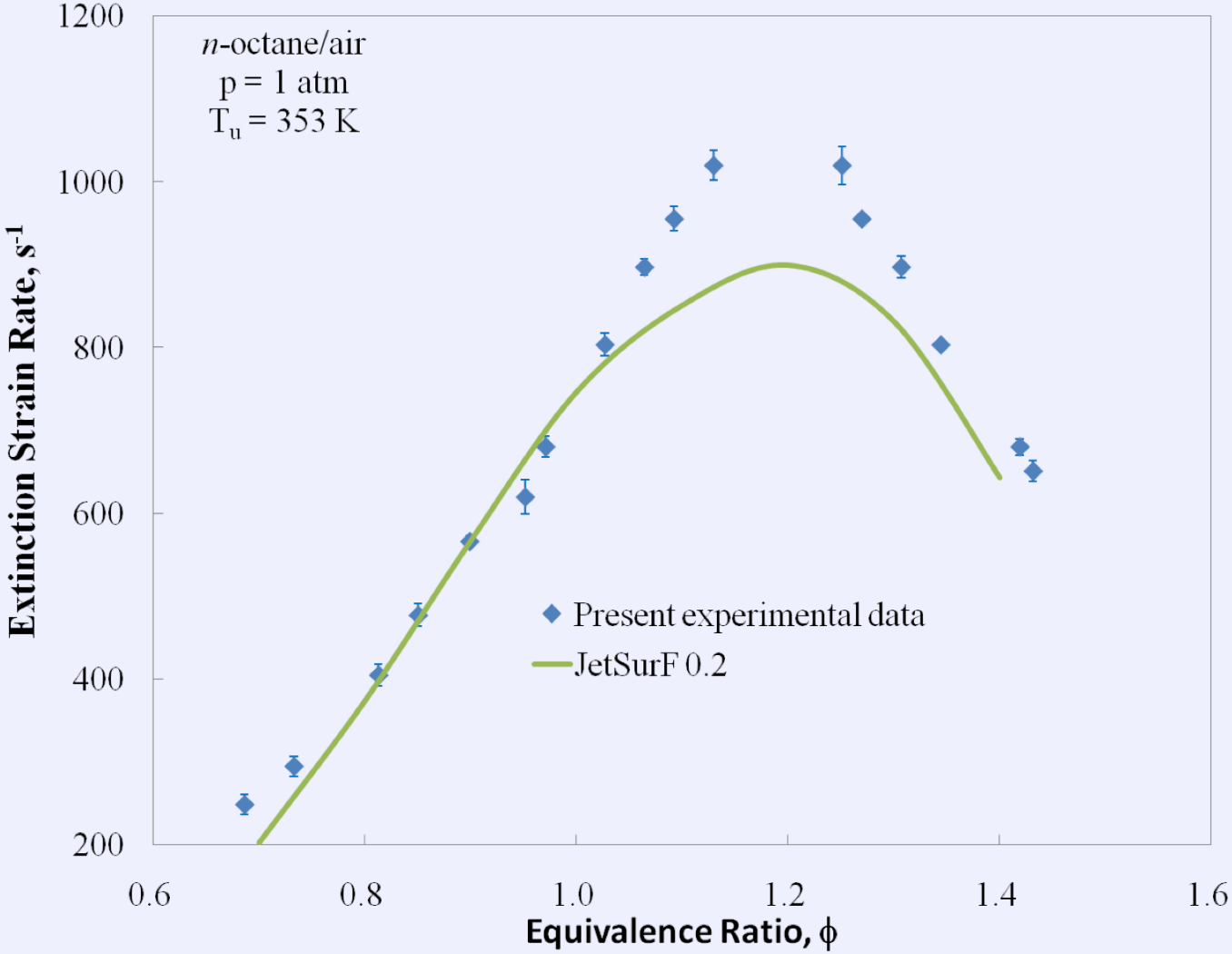
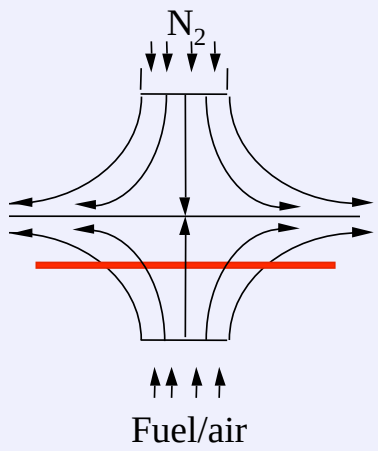
Extinction Strain Rates of n-Octane/Air Flames[1]





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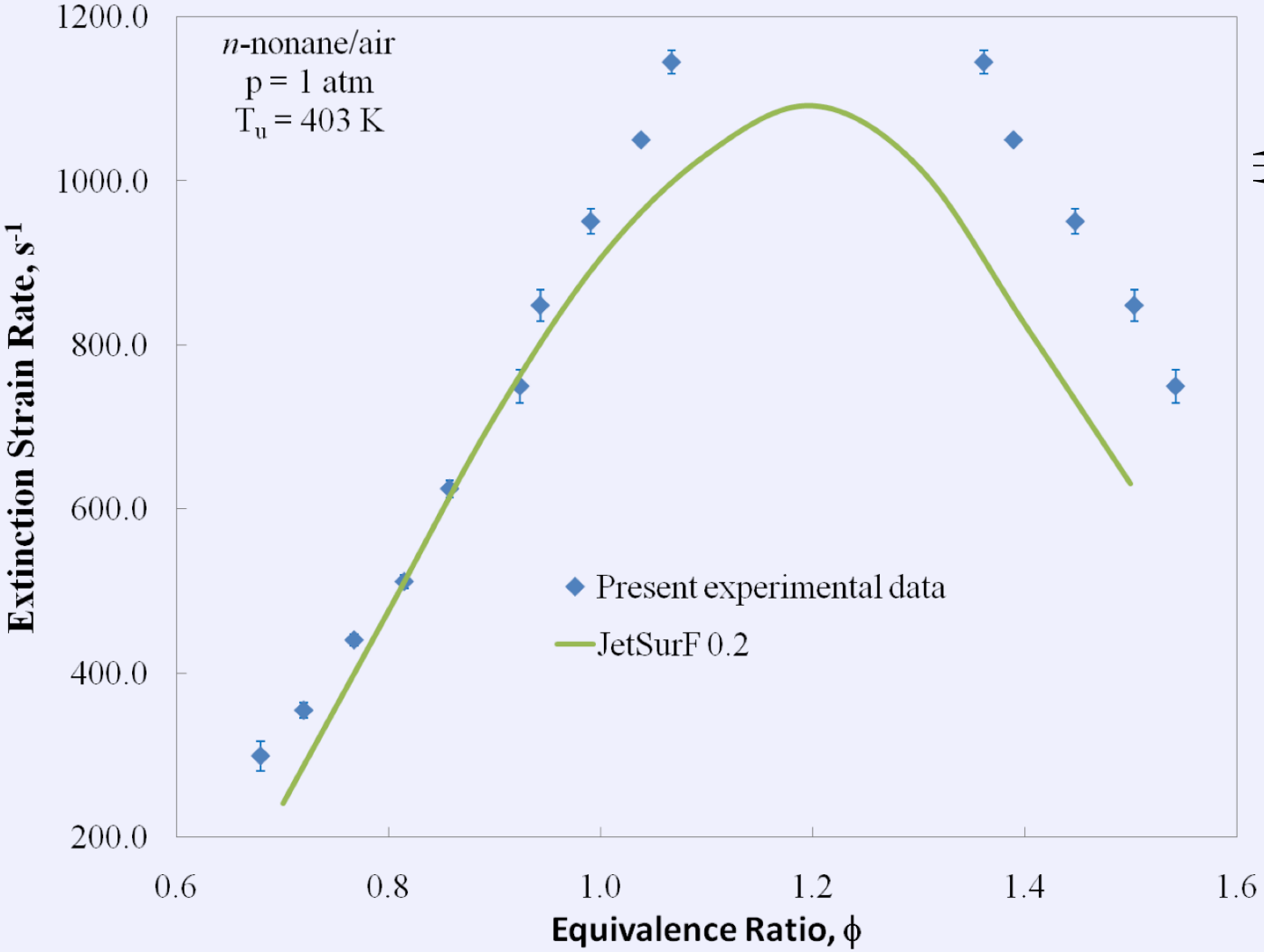
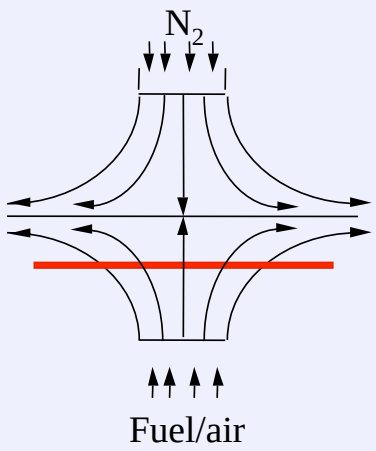
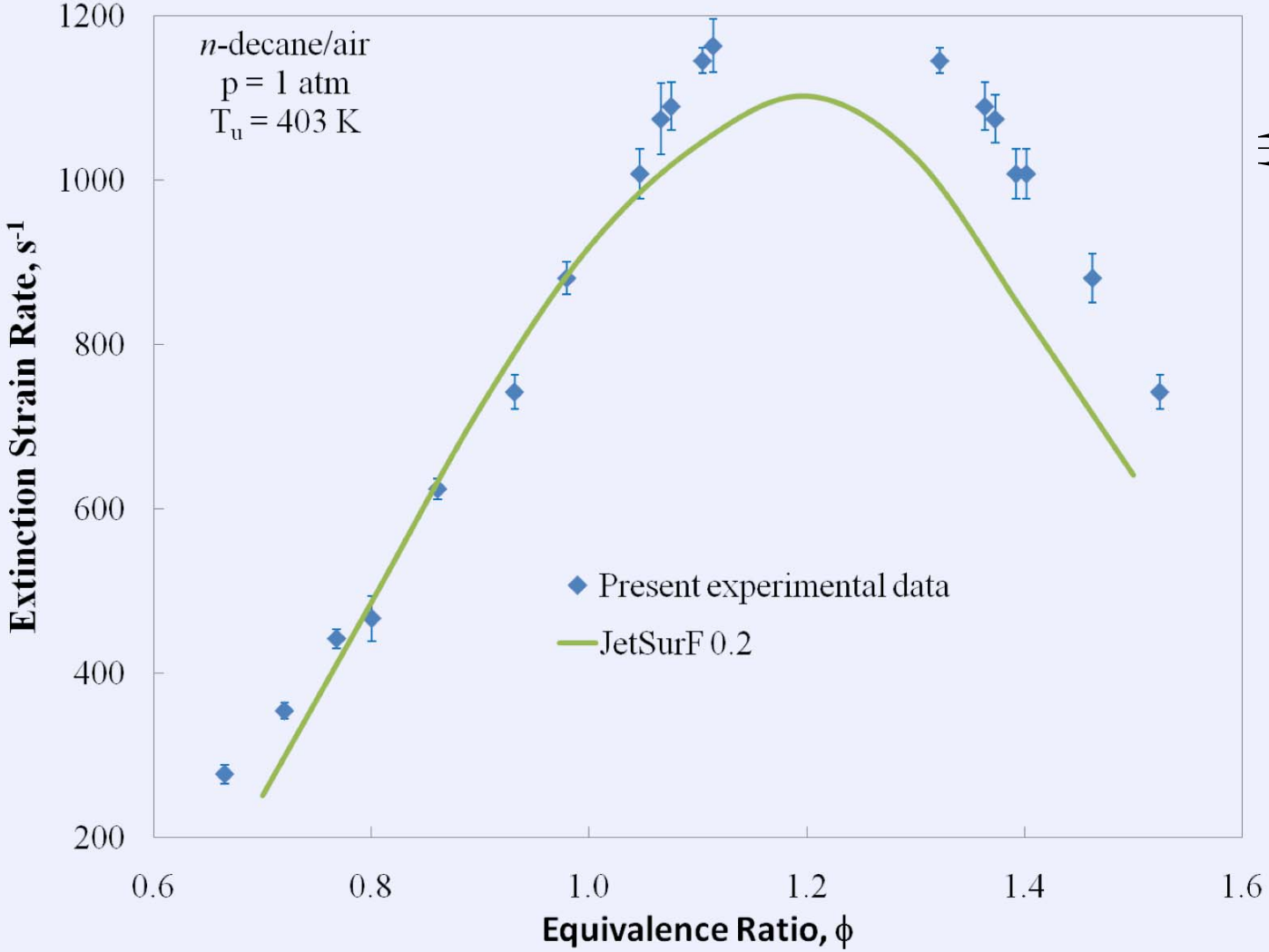
Extinction Strain Rates of n-Nonane/Air Flames[1]

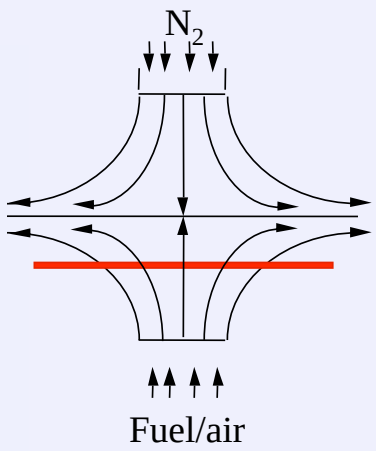




[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

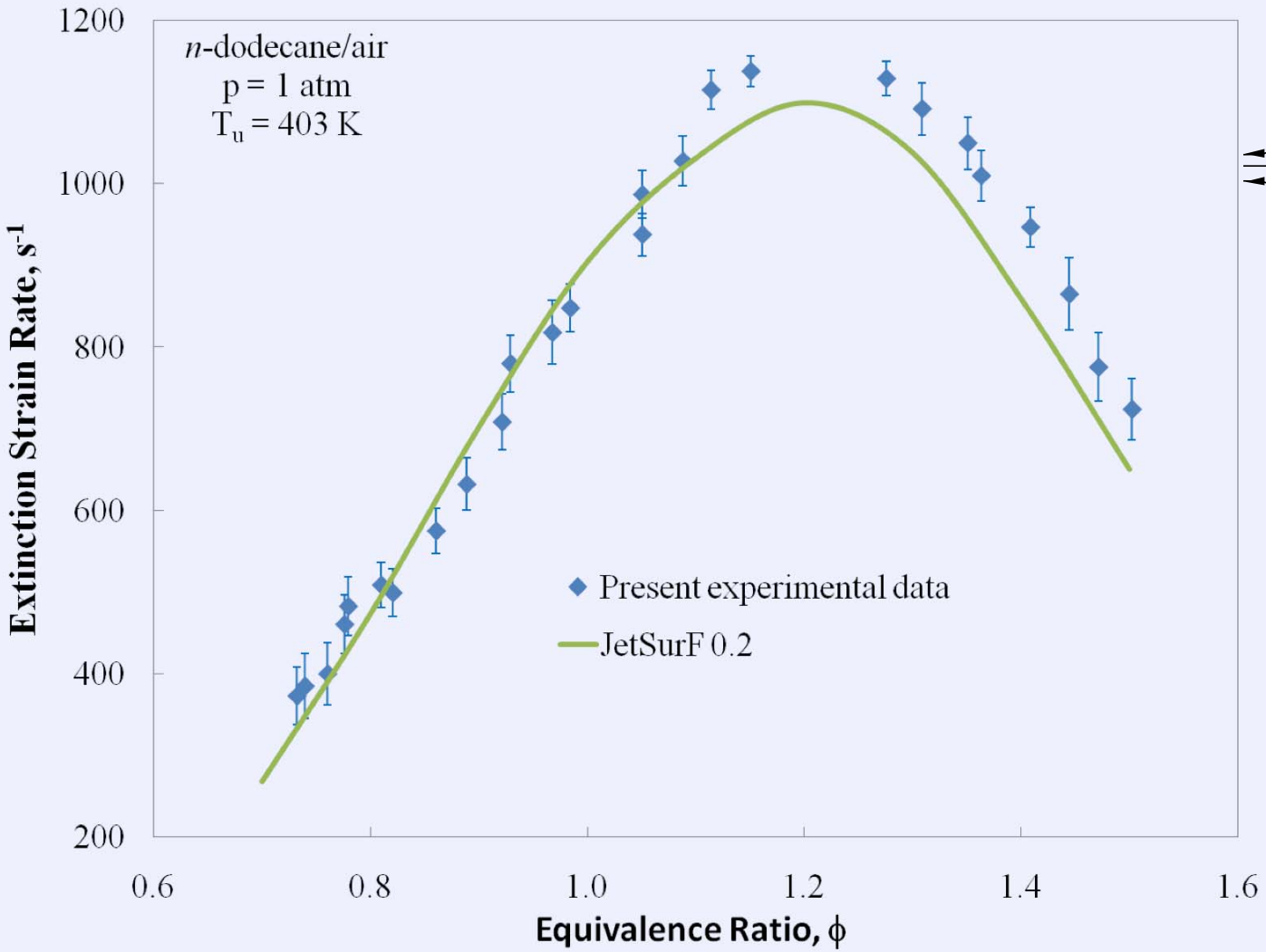
Extinction Strain Rates of n-Decane/Air Flames[1]

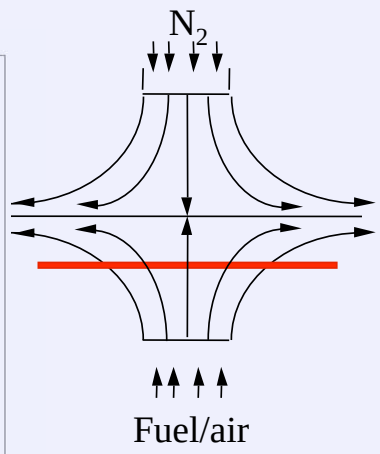




[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

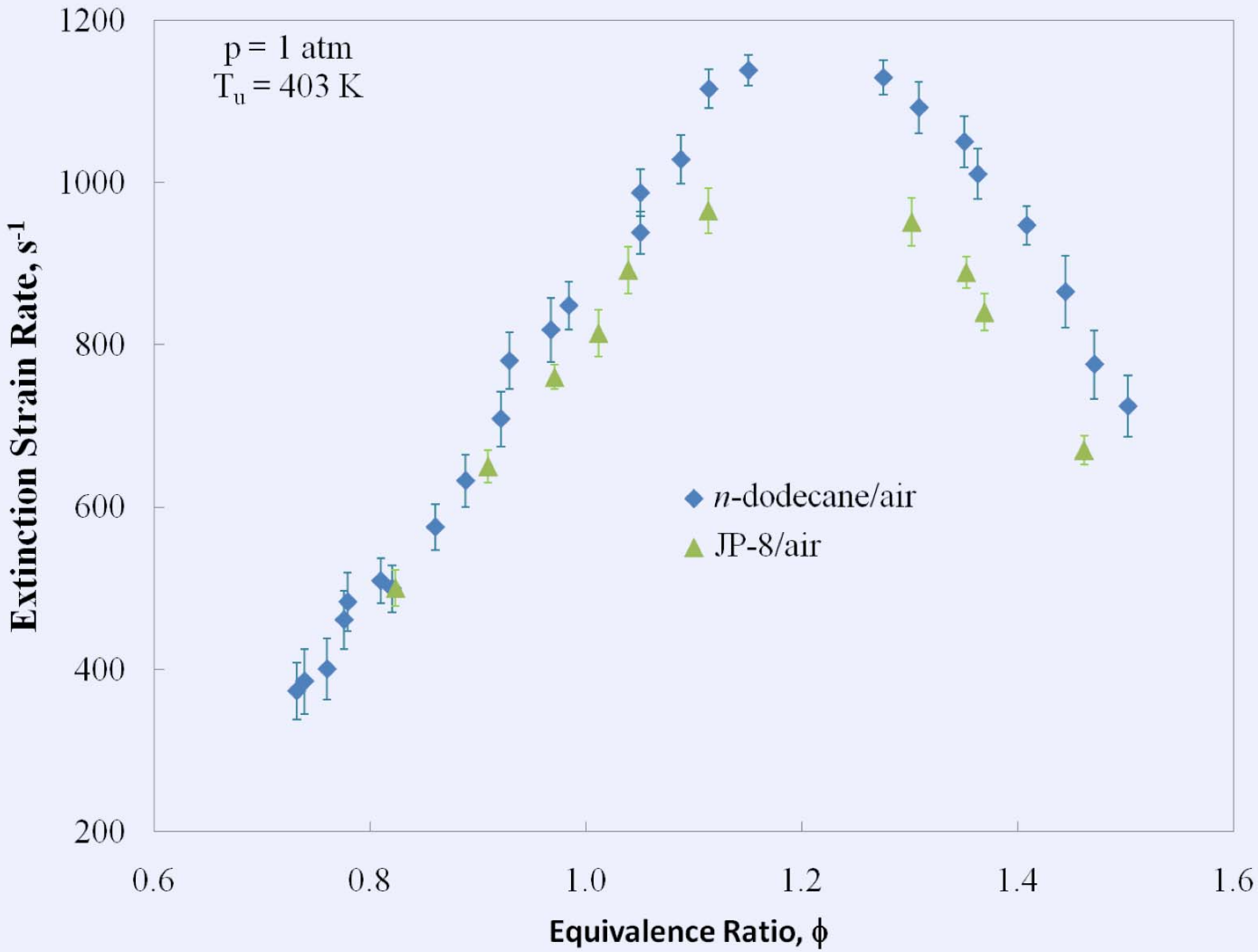
Extinction Strain Rates of n-Dodecane/Air Flames[1]

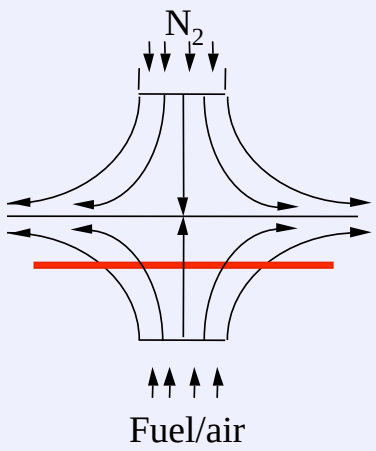




[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Flame Extinction: n-Dodecane vs. JP-8[1]



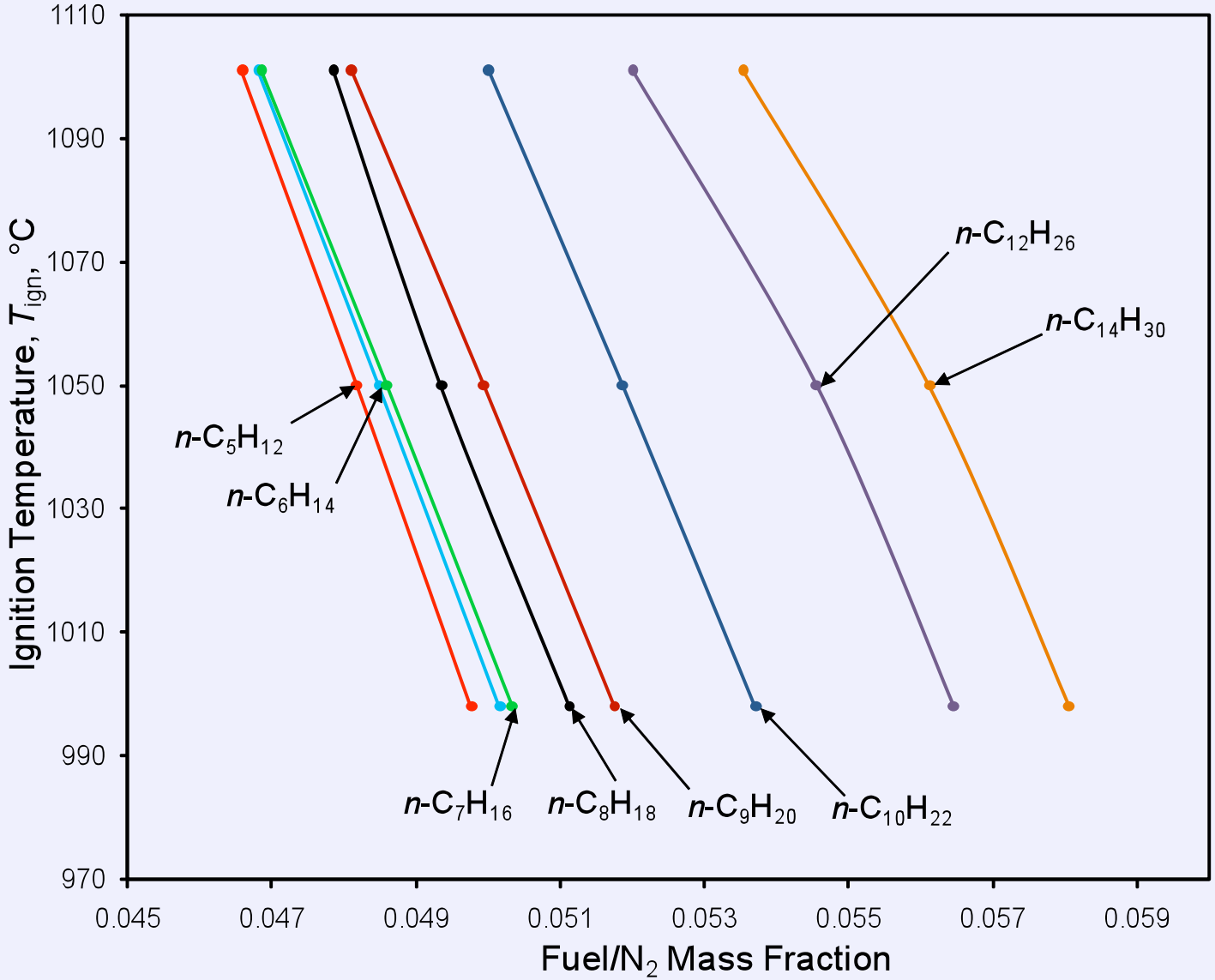


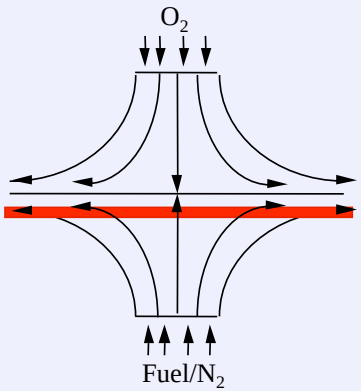
[1]C. Ji, A.T Holley, F.N. Egolfopoulos, unpublished data (2008)

Sensitivity of Properties of Large Hydrocarbon Flames to Reactant Diffusion[5]

[5]**A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)**

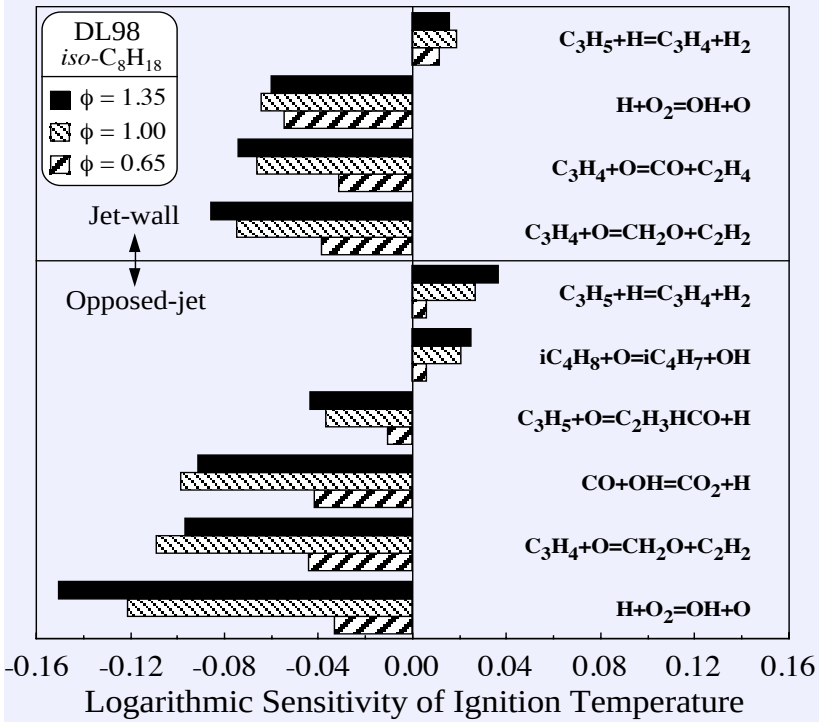
Effect of Fuel Size on Flame Ignition[6]

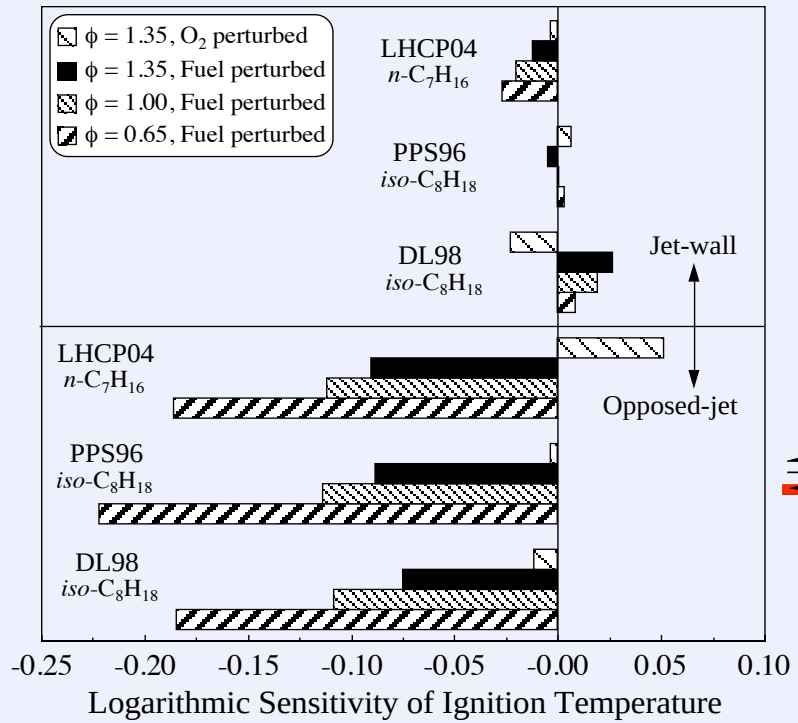


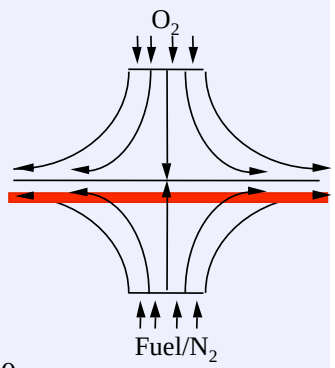


[6]A.T. Holley, Y. Dong, M.G. Andac, F.N. Egolfopoulos, and T. Edwards, *Proceedings of the Combustion Institute* 31: 1205-1213 (2007)

Effect of Fuel Size on Flame Ignition[7]



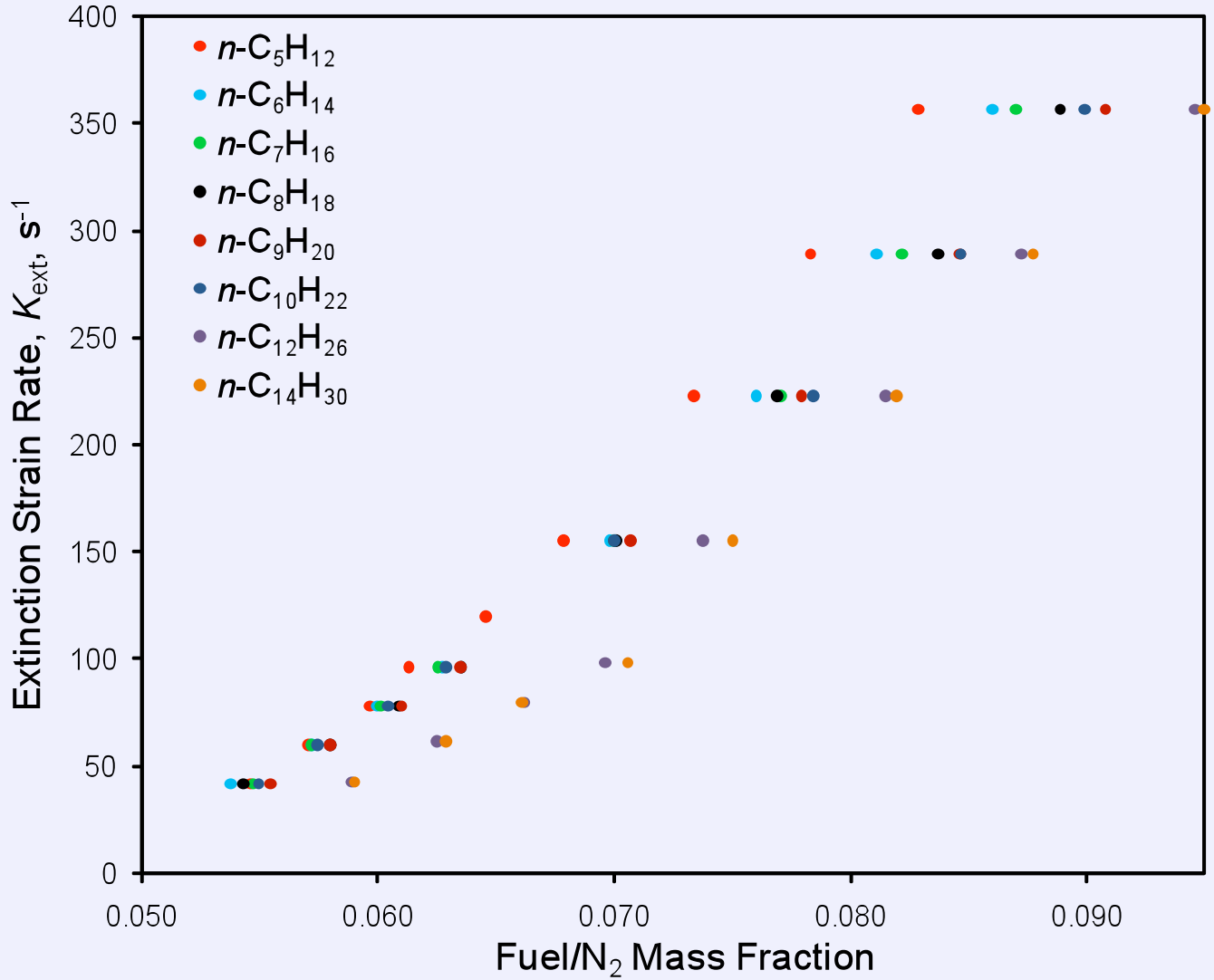


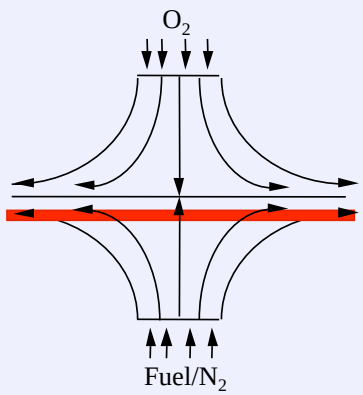


Kinetics **Diffusion**

[7]M.G. Andac, F.N. Egolfopoulos, *Proceedings of the Combustion Institute* 31: 1165-1172 (2007)

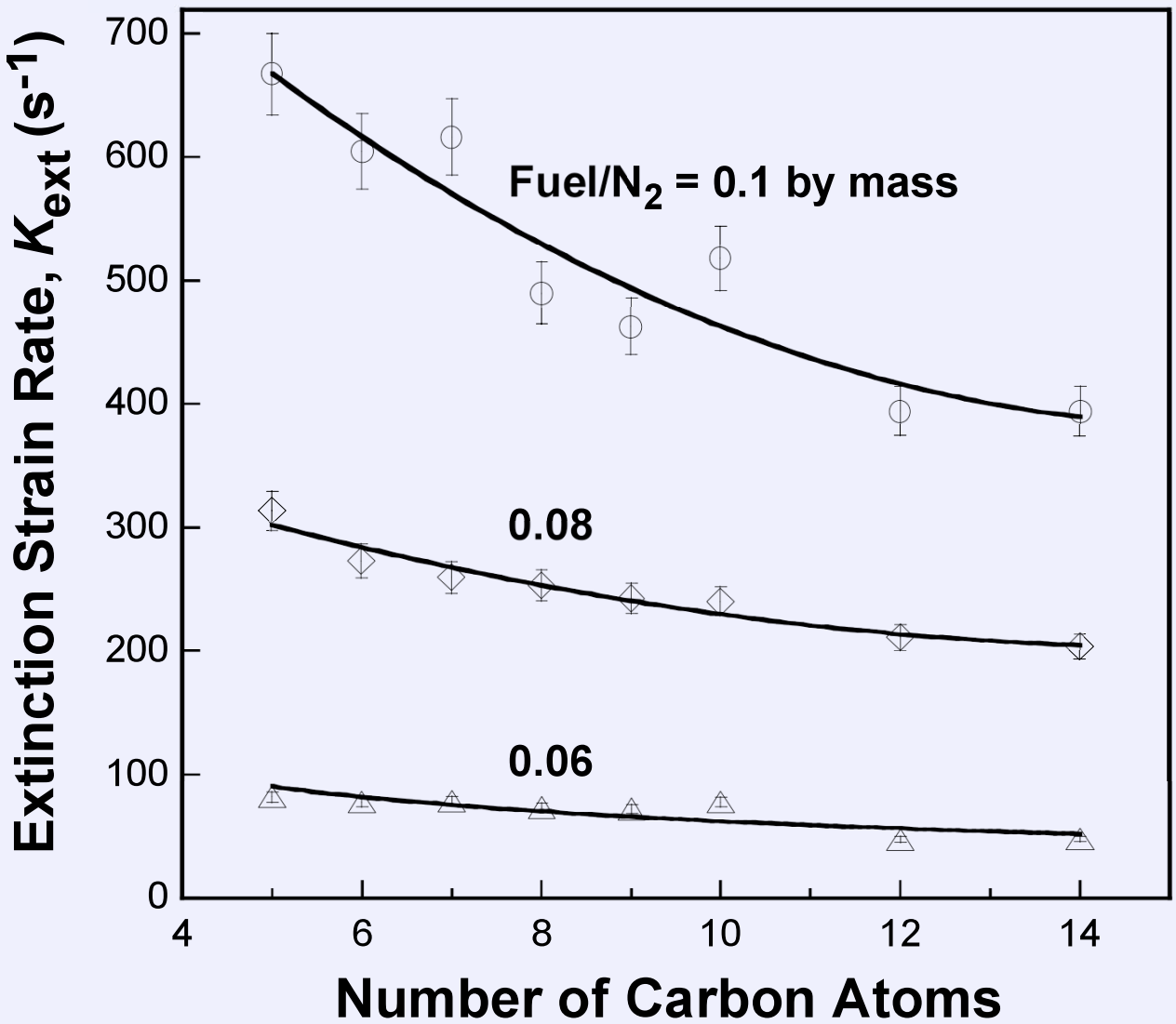
Effect of Fuel Size on Flame Extinction[6]

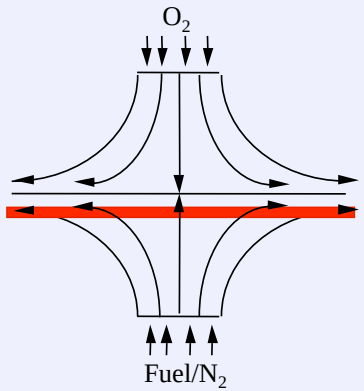




[6]A.T. Holley, Y. Dong, M.G. Andac, F.N. Egolfopoulos, and T. Edwards, *Proceedings of the Combustion Institute* 31: 1205-1213 (2007)

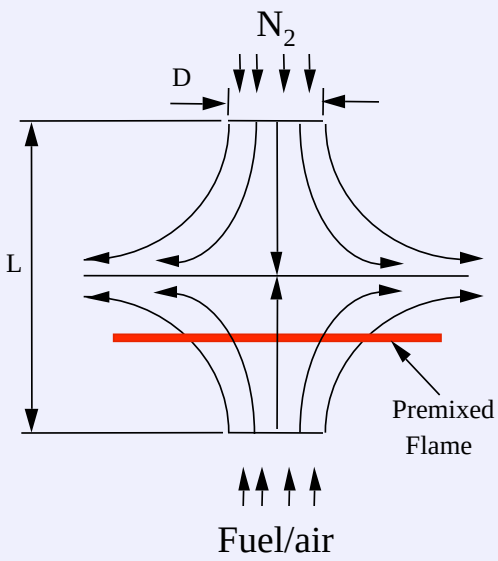
Effect of Fuel Size on Flame Extinction[6]

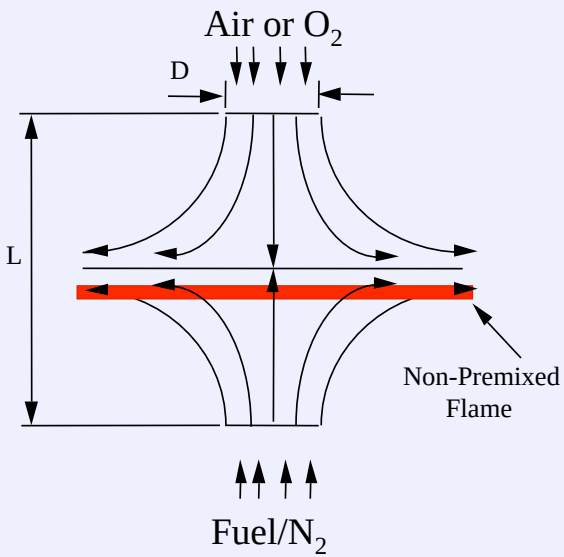




[6]A.T. Holley, Y. Dong, M.G. Andac, F.N. Egolfopoulos, and T. Edwards, *Proceedings of the Combustion Institute* 31: 1205-1213 (2007)

Flame Configurations Considered[5]

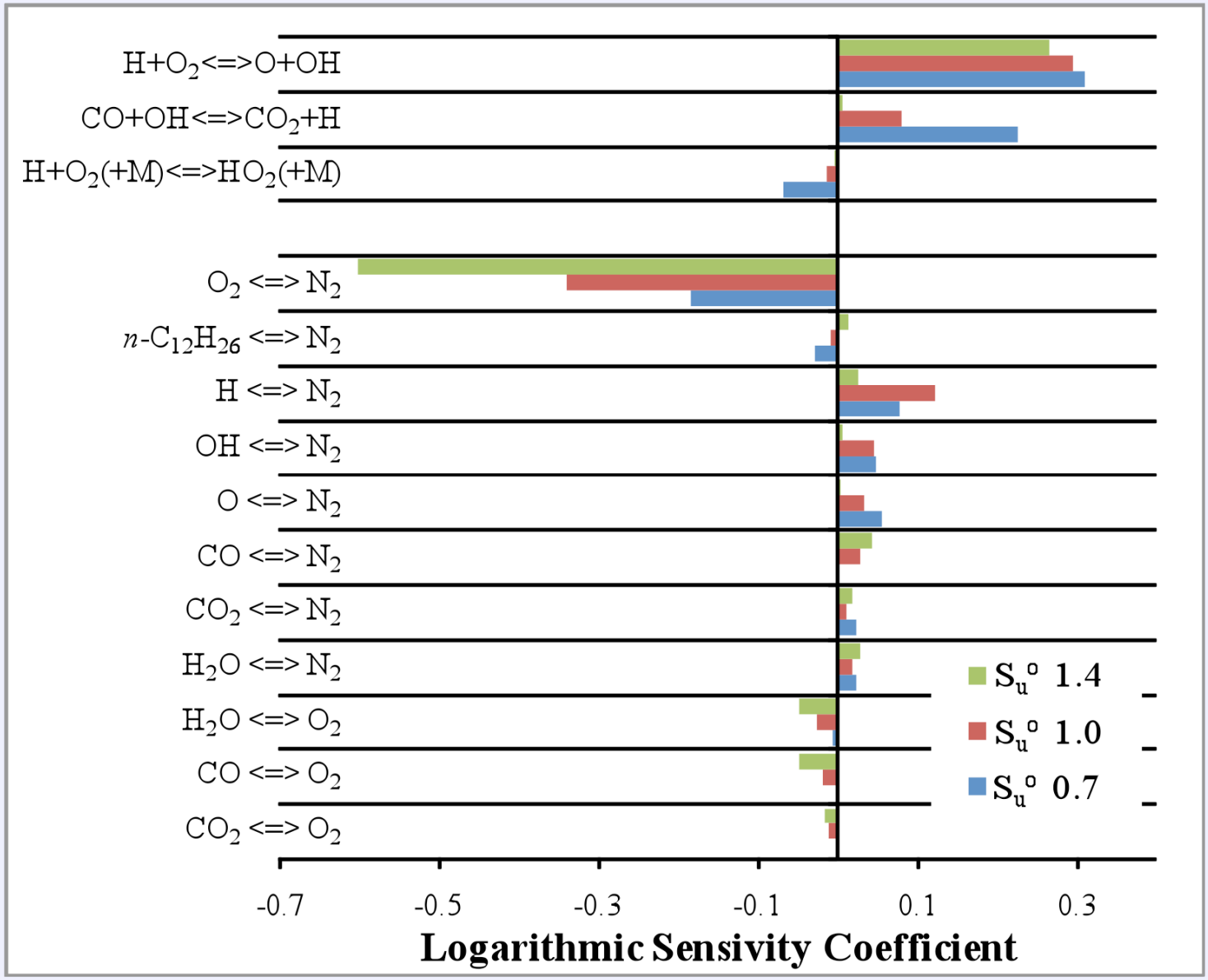




Flame	Description
Laminar Flame Speed (T_u = 403 K)	
S_u° 1.4	ϕ=1.4
S_u° 1.0	ϕ=1.0
S_u° 0.7	ϕ=0.7
Extinction strain rate of premixed flame	
K_{ext} 1.4	Fuel/air (ϕ=1.4) vs. N_2
K_{ext} 1.0	Fuel/air (ϕ=1.0) vs. N_2
K_{ext} 0.7	Fuel/air (ϕ=0.7) vs. N_2
Extinction strain rate of nonpremixed flame	
K_{ext} 1:30 (air)	Fuel/ N_2=1/30 vs. Air
K_{ext} 1:15 (air)	Fuel/ N_2=1/15 vs. Air
K_{ext} 1:120 (O_2)	Fuel/ N_2=1/120 vs. O_2
K_{ext} 1:60 (O_2)	Fuel/ N_2=1/60 vs. O_2

[5]**A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)**

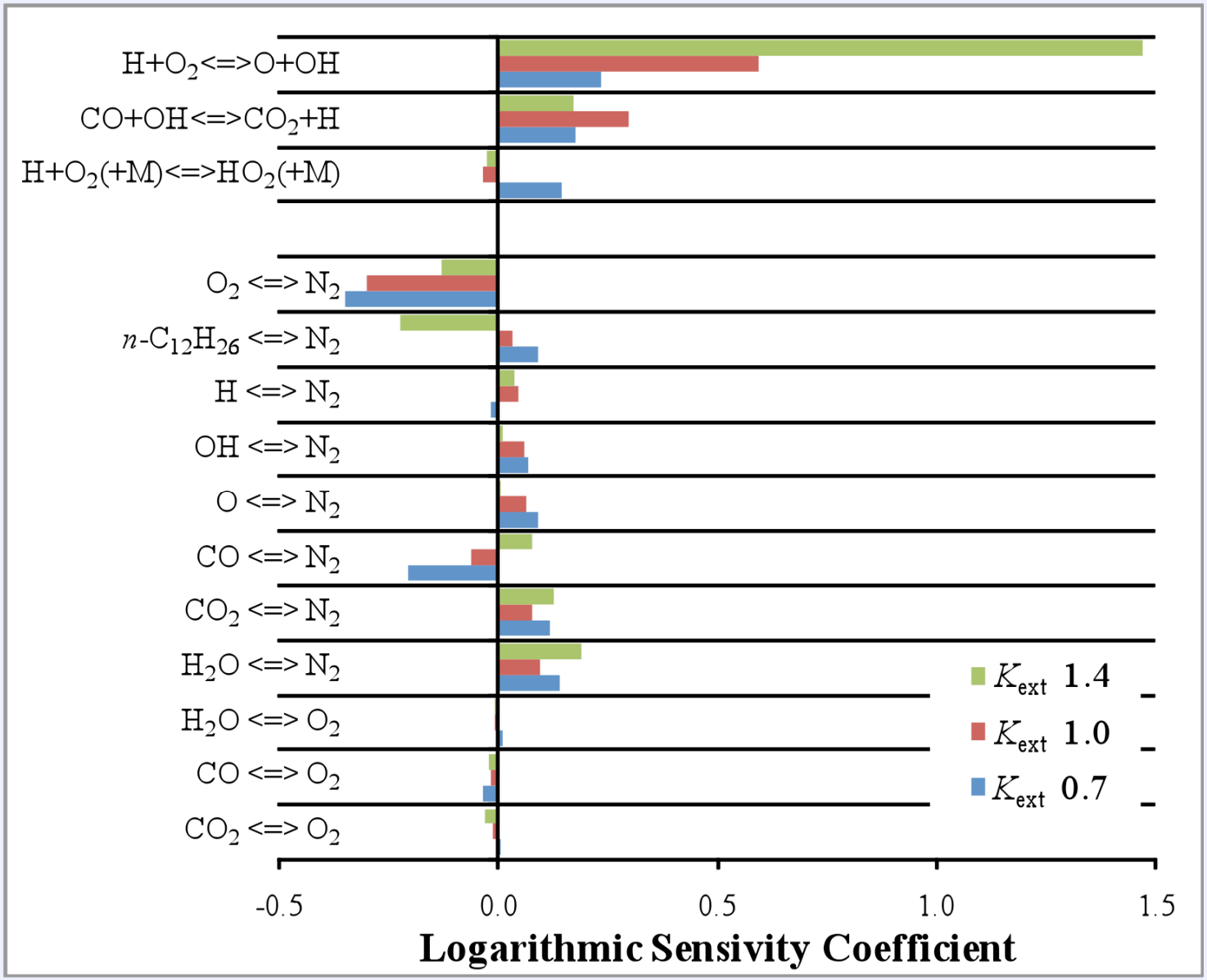
Sensitivity of Laminar Flame Speed on Kinetics/Transport[5]

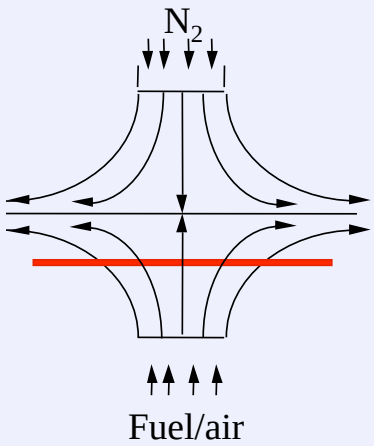


***n*-dodecane/air**
p=1 atm
T_u=403 K

[5]A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

Sensitivity of Extinction (Premixed) on Kinetics/Transport[5]

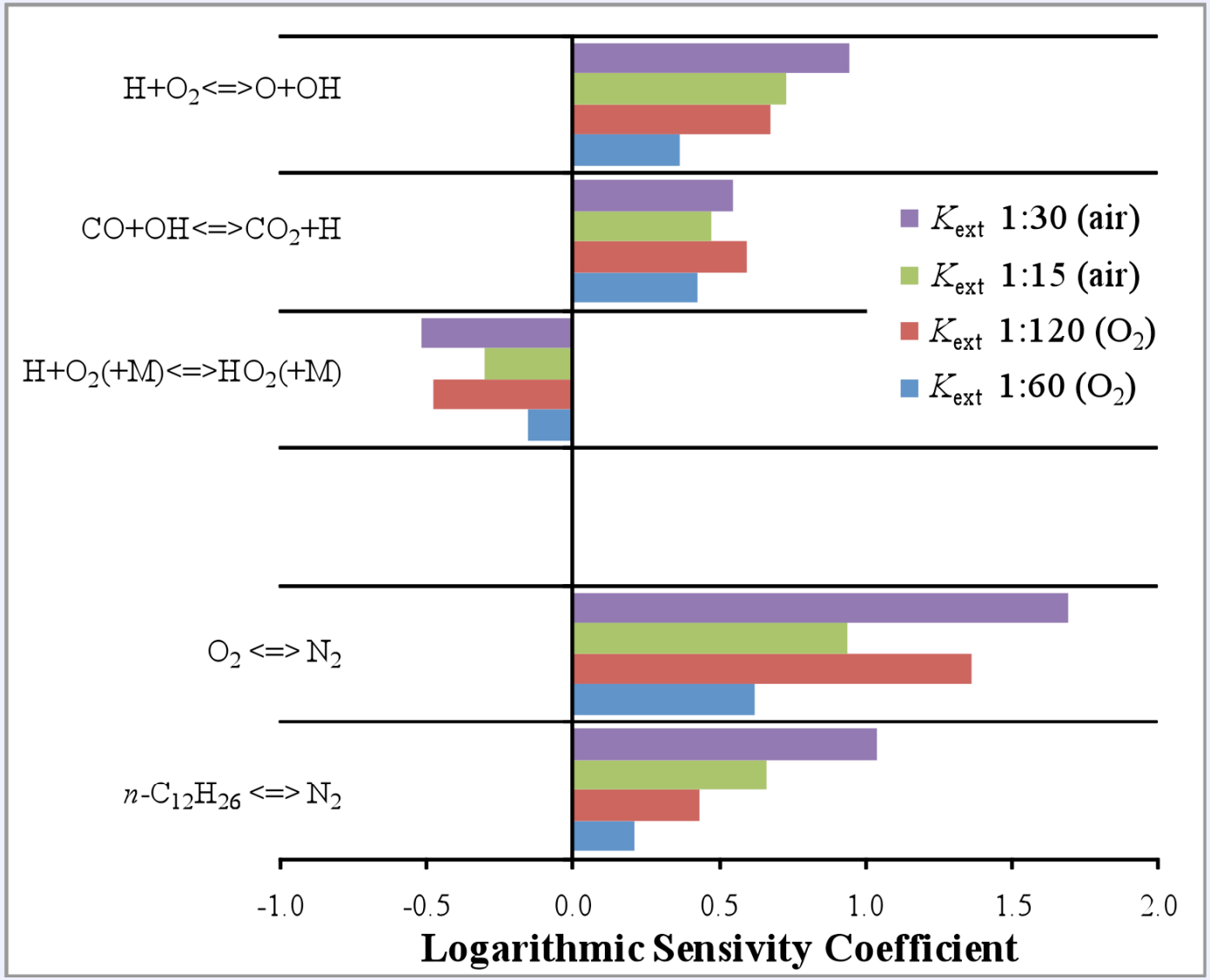


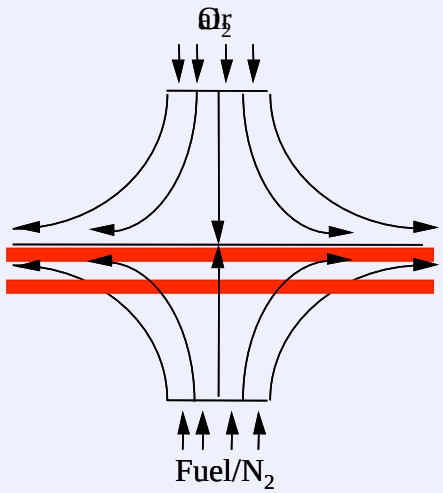


***n*-dodecane/air**
p=1 atm
T_u=403 K

[5]A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

Sensitivity of Extinction (Non-Premixed) on Kinetics/Transport[5]

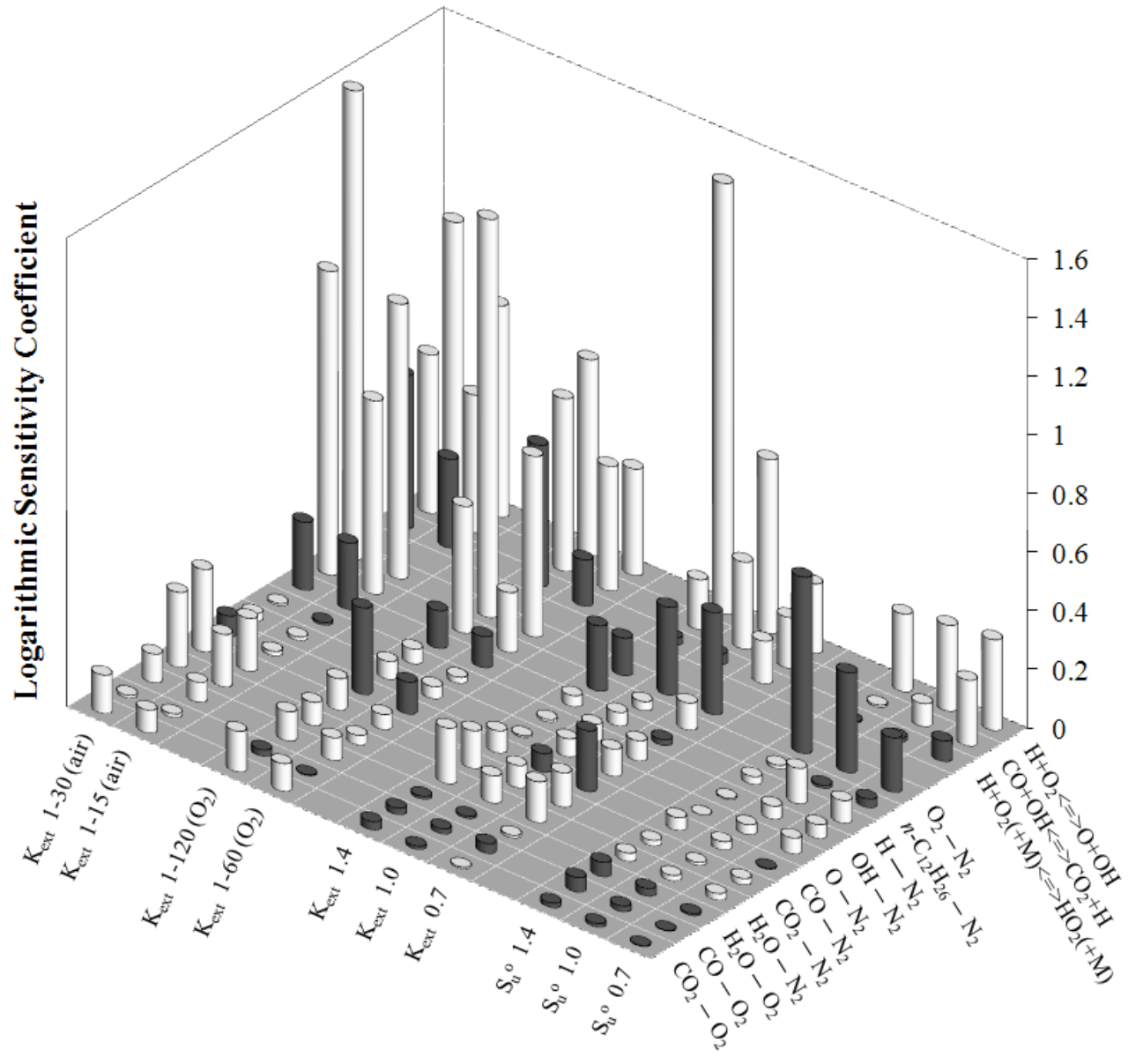




***n*-dodecane**
p=1 atm
T_u=403 K

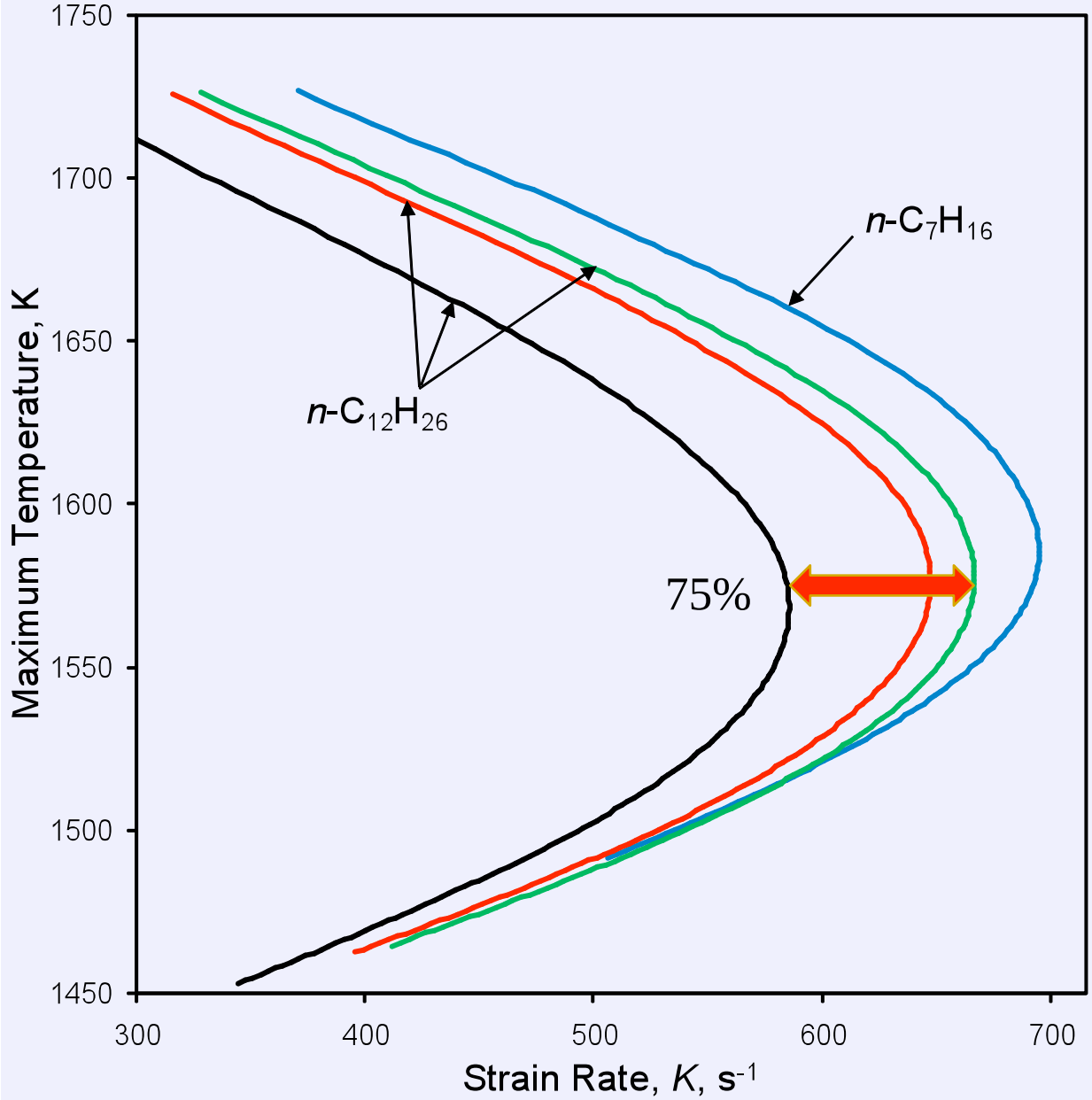
[5]A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

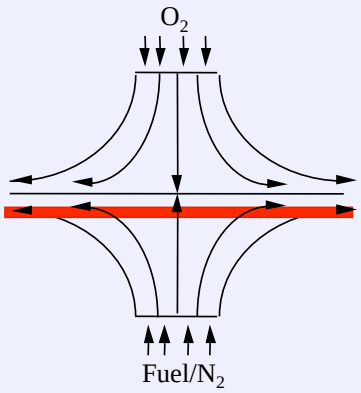
Sensitivity of All Phenomena Considered on Kinetics/Transport[5]



[5]A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

Kinetics vs. Transport Contribution to Extinction (Non-Premixed)[5]





- **Non-premixed flame extinction curves for n-C_7H_{16} and n-$C_{12}H_{26}$ with fuel/N_2 mass ratio of 0.08 against an O_2 jet.**
- **The three n-$C_{12}H_{26}$ cases are:**
  - **Black - base case**
  - **Red - the BDC of n-$C_{12}H_{26}$-N_2 replaced by that of n-C_7H_{16}-N_2**
  - **Green - all BDC of n-$C_{12}H_{26}$ replaced by n-C_7H_{16}**

[5]A.T. Holley, X.Q. You, E. Dames, H. Wang, F.N. Egolfopoulos, to appear in *Proceedings of the 32nd International Symposium on Combustion* (2008)

Concluding Remarks

1. **A new approach has been advanced to determine laminar flame speeds of large hydrocarbon flames.**
2. **Laminar flame speeds were found to differ under rich conditions from recent measurements and be within 5-15% of those of JP-8/air mixtures.**
3. **Extinction strain rates of *n*-dodecane/air mixtures were found to be also within 5-15% of those of JP-8/air mixtures.**
4. **A *n*-dodecane mechanism has been advanced and tested against the experimental data and close agreements were found.**
5. **The effect of binary diffusion coefficients on flame propagation and extinction was rigorously quantified.**
6. **Under certain conditions the effect of diffusion on the flame response is of the same magnitude with that of kinetics.**
7. ***Flame experiments require particular care to overcome inherent challenges and model validation must account for both kinetics and transport effects***