Multi Agency Coordination Committee for Combustion Research (MACCCR)
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Extinction of Non-Premixed Undiluted-Hydrocarbons vs. Air Counterflow Flames: Comparisons on an "Absolute" Axial-Strain-Rate Scale

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Overview of Presentation

- OJB Extinction Limits Mimic “Idealized” Scramjet Flameholding
- Experimental Approach; and Extinction Data for C_1 to C_4 HCs
- Determination of Gaseous Surrogate HC Fuel for HIFiRE
- Effects of O_2 (and NO) Concentration on HC Extinction
- Results from Convergent-Nozzles and Straight-Tube OJBs; Transformation of Global Strain Rates; and Comparisons.
- Summary Extinction of Non-Premixed, Undiluted-HCs vs. Air; 7 C_1 to C_4 Gaseous HCs, & 11 Vaporized HCs up to n-$C_{14}H_{30}$.

Use of OJB Extinction Limits to Mimic "Idealized" Scramjet Flame-Holding Limits, and Define a Simple Gaseous Surrogate Fuel

- **HIFiRE Flight 2**
  - Hypersonic International Flight Research Experiment. Participants are: NASA Langley; U.S. Air Force AFRL; ATK Alliant Tech Systems; and the Australian Defence Science and Tech Org., DSTO.
  - **Flight Goal:** To demonstrate dual-mode to scramjet performance transition, using a gaseous hydrocarbon surrogate fuel that mimics ignition and flame holding properties of a catalytically-cracked JP-7 "like" kerosene.

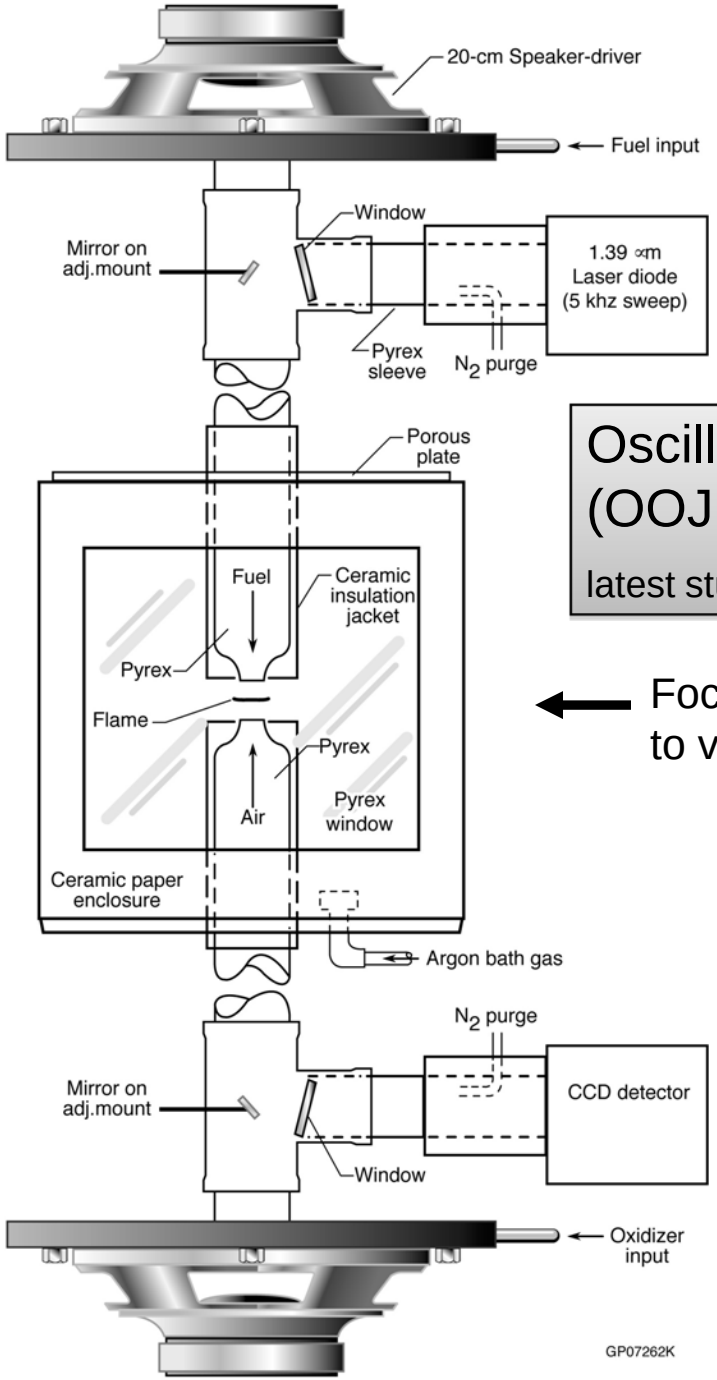
Experimental Approach

and

Extinction Data for Non-Premixed C_1 to C_4 HCs vs. Air

Extinction / Flameholding Performance Gauges

- **Opposed Jet Burner Extinction Limits:**
  - ★ **Flame Strength [FS = cross-section-average U_{air} (MF) at nozzle exit].**
  - ★ **FSs measure aerodynamically-strained, non-premixed combustion limits at T's relevant to flameholding in simple systems**.
- **Applied Stress Rate (ASR) Extinction Limits** (after Spalding, Dixon-Lewis)
  - ★ **ASRs at extinction represent jet-diameter-normalized FSs for convergent nozzles (plug inflow) and uniform tubes (parabolic).**
  - ★ **ASR limits define reproducible global scales for fuel–air systems (primarily influenced by chemical kinetics *and* diffusion).**
  - ★ **Limits enable a *relative* assessment of incipient flameholding (flameout) in scramjet (e.g., in subsonic recirculation zone).**
  - ★ **ASRs allow validation of kinetics & multi-component diffusion.**



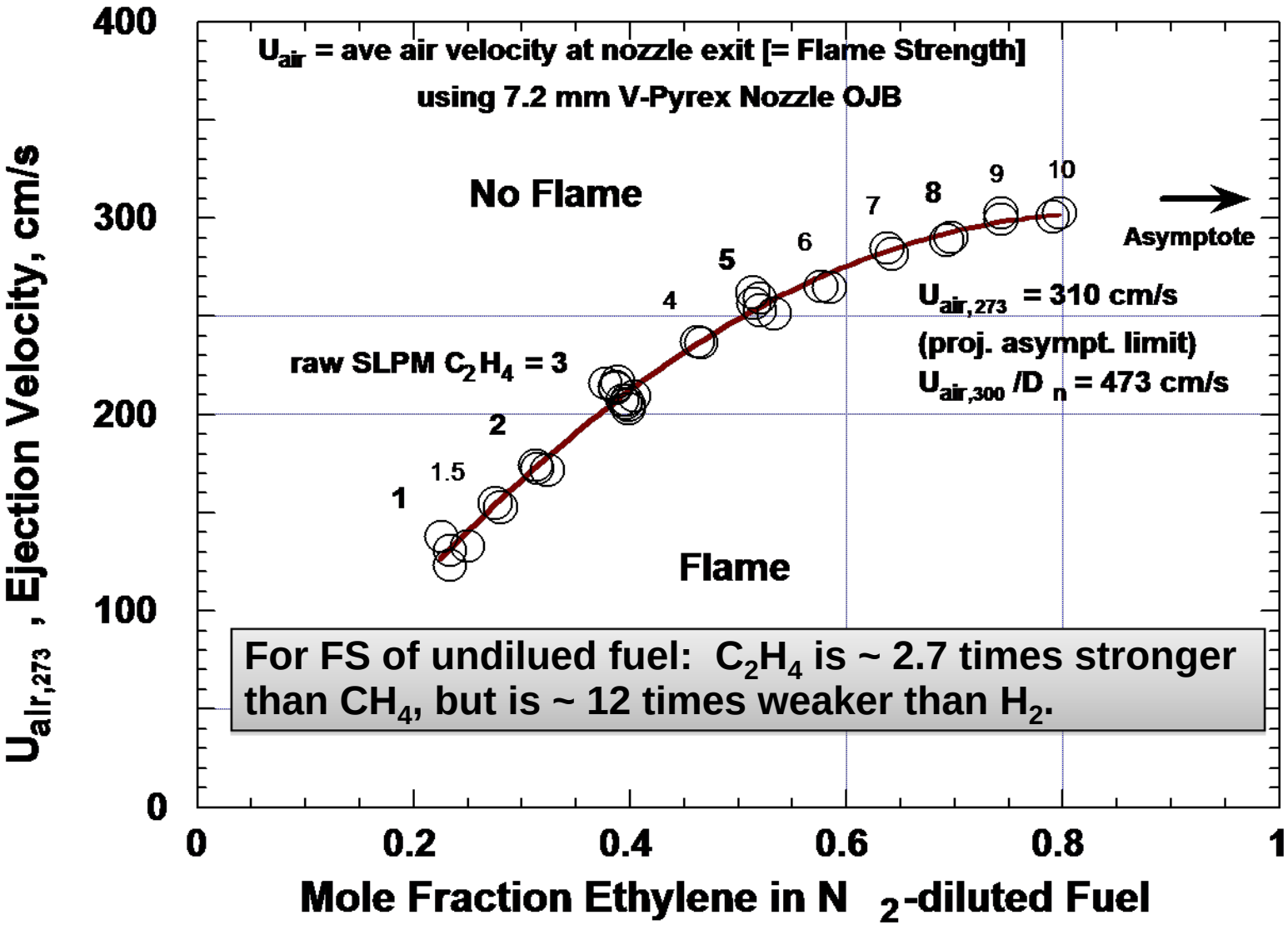
Diode laser system is passive in this study

Oscillatory-input Opposed Jet Burner (OOJB) System

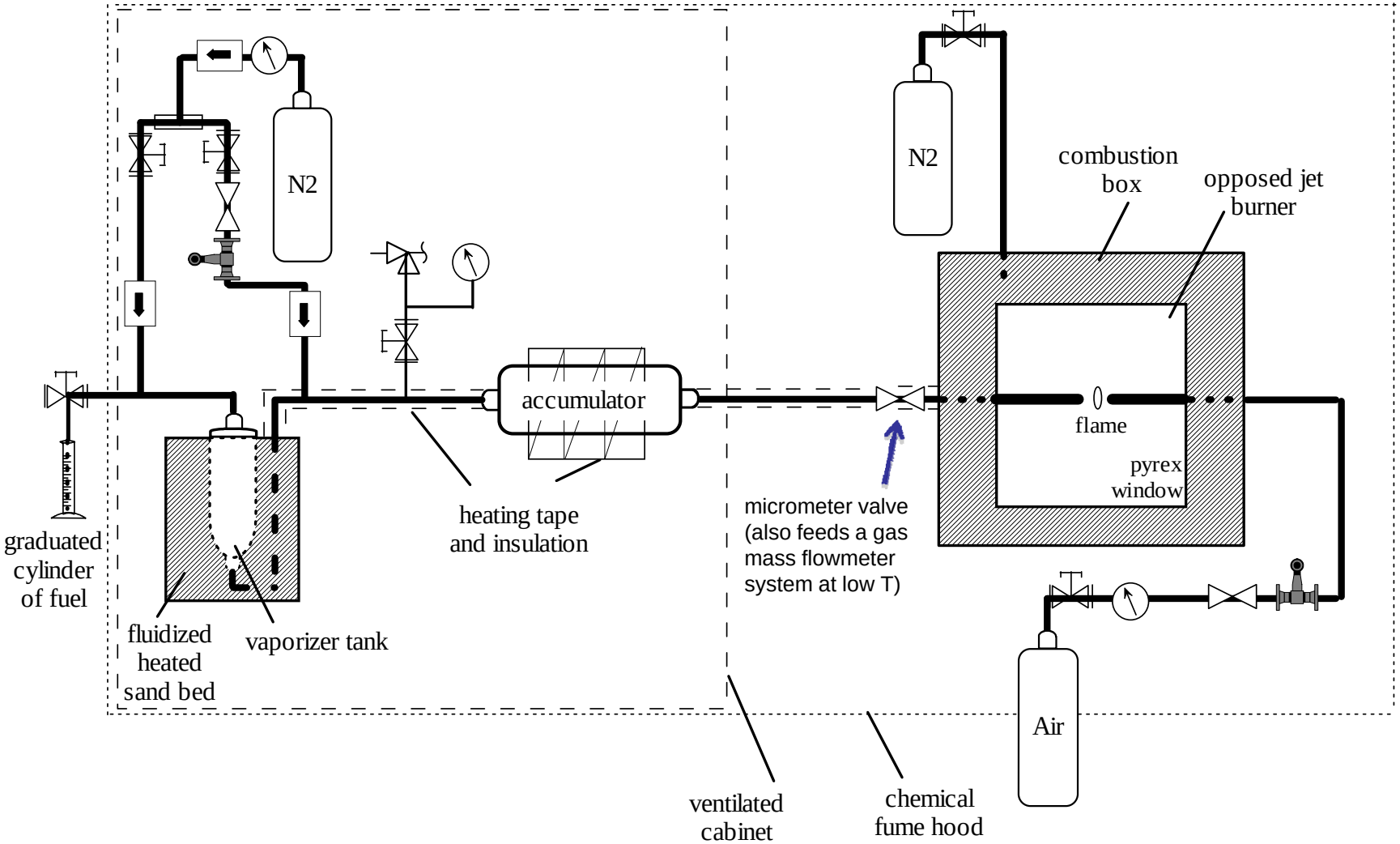
(used for "steady" extinction; latest study of unsteady extinction, AIAA 2009-4879)

Focusing Schlieren System to visualize flame structure

Steady-State Extinction of C_2H_4/N_2—Air Counterflow Diffusion Flames using 7.2 mm V-Pyrex Nozzle OOJB

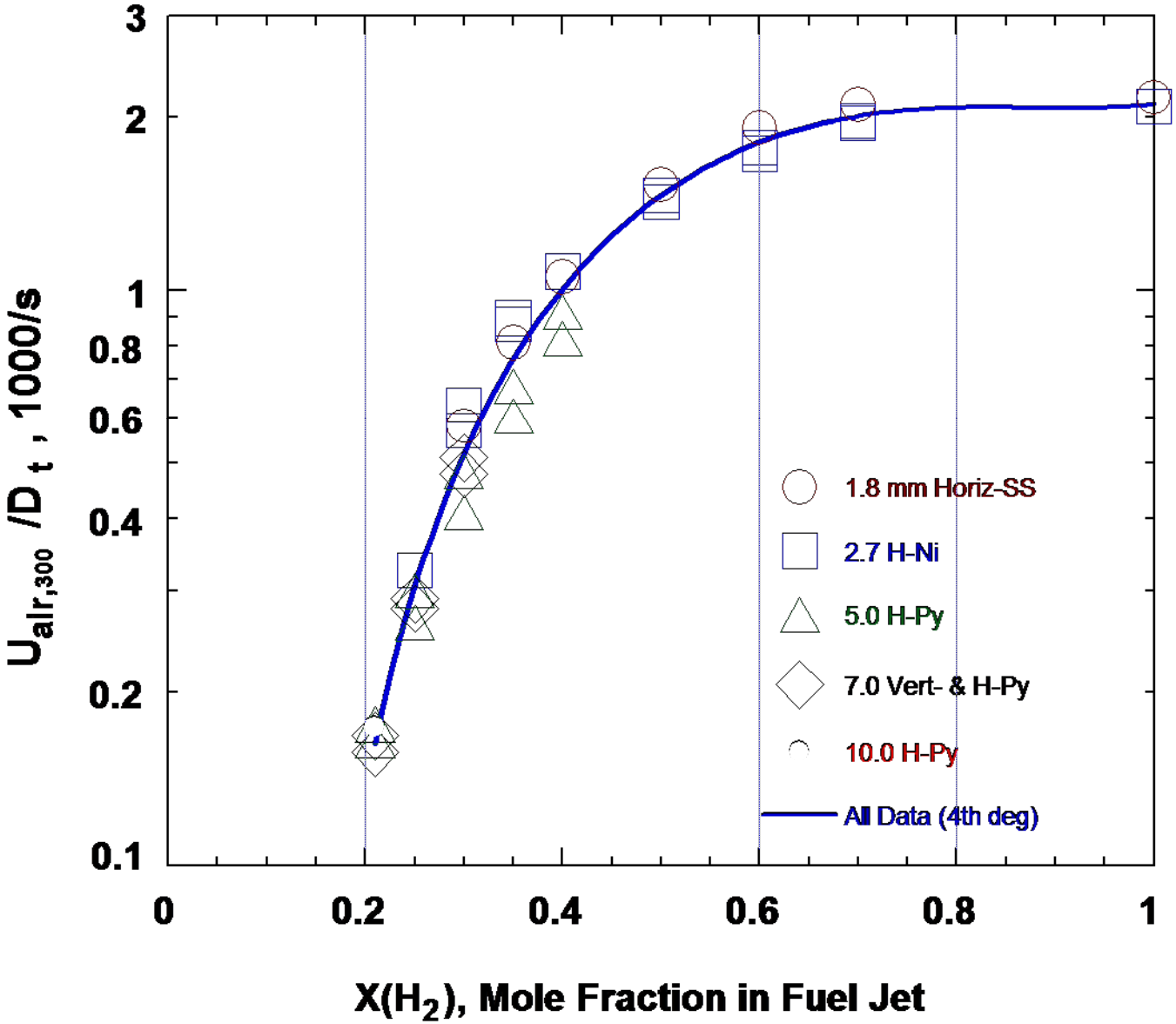


For FS of undilued fuel: C_2H_4 is ~ 2.7 times stronger than CH_4, but is ~ 12 times weaker than H_2.

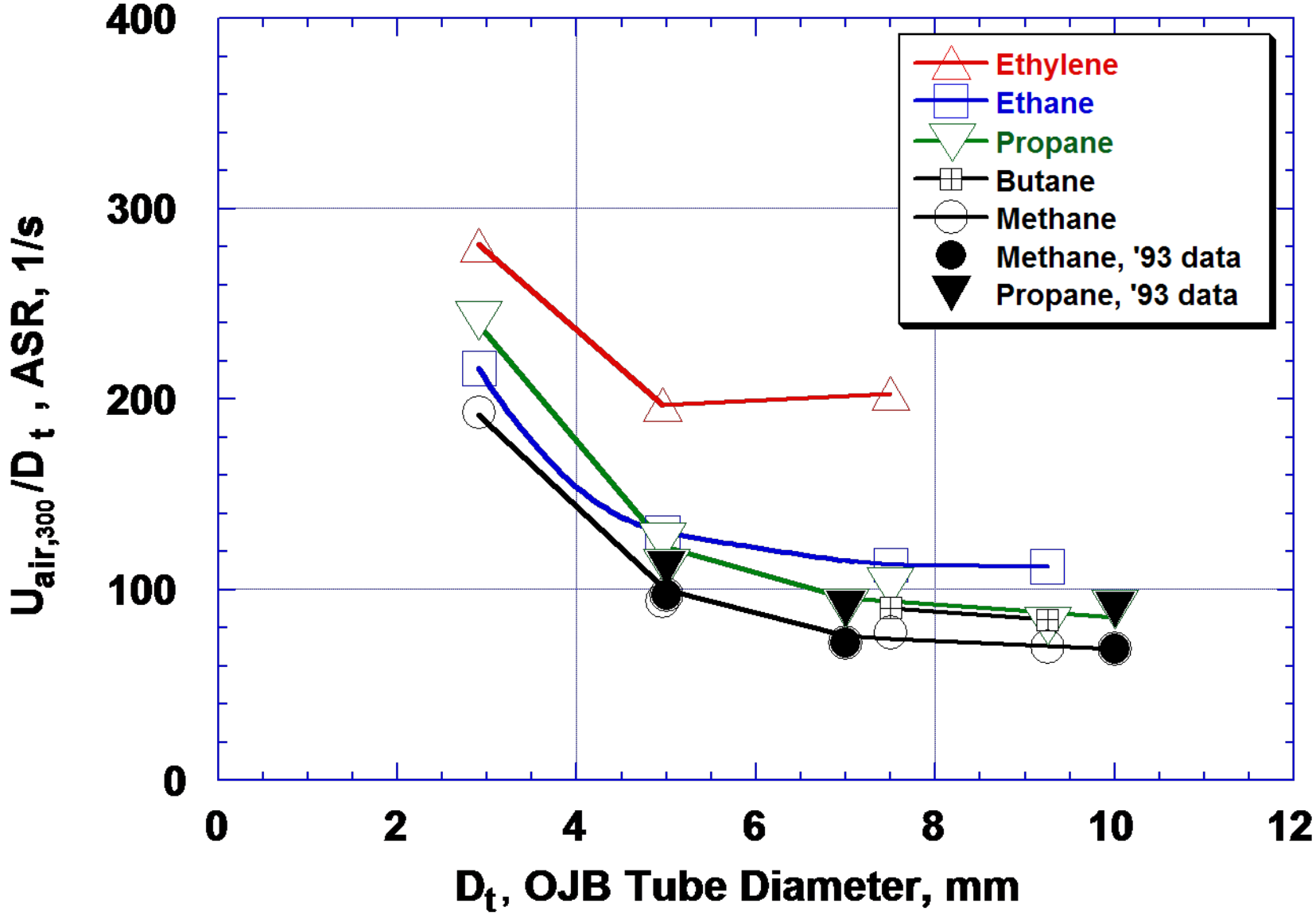


Liquid-Fuel Vaporizer, and Various-size Horizontal-Tube Opposed Jet Burners (1 atm)

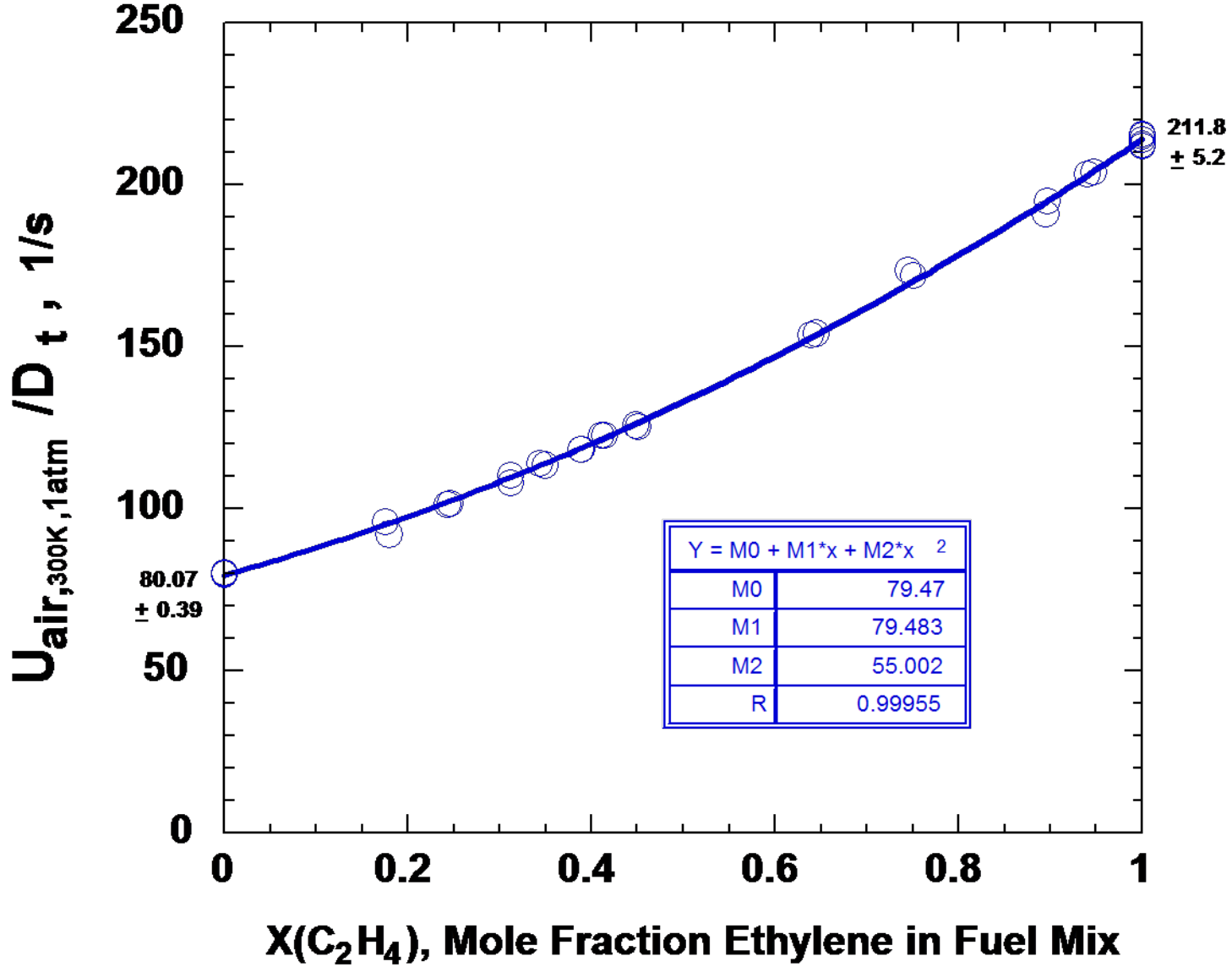
Applied Stress Rate for Tube-OJBs "at 300 K Airside Edge of Flame," for Extinction of H_2/N_2—Air CFDFs



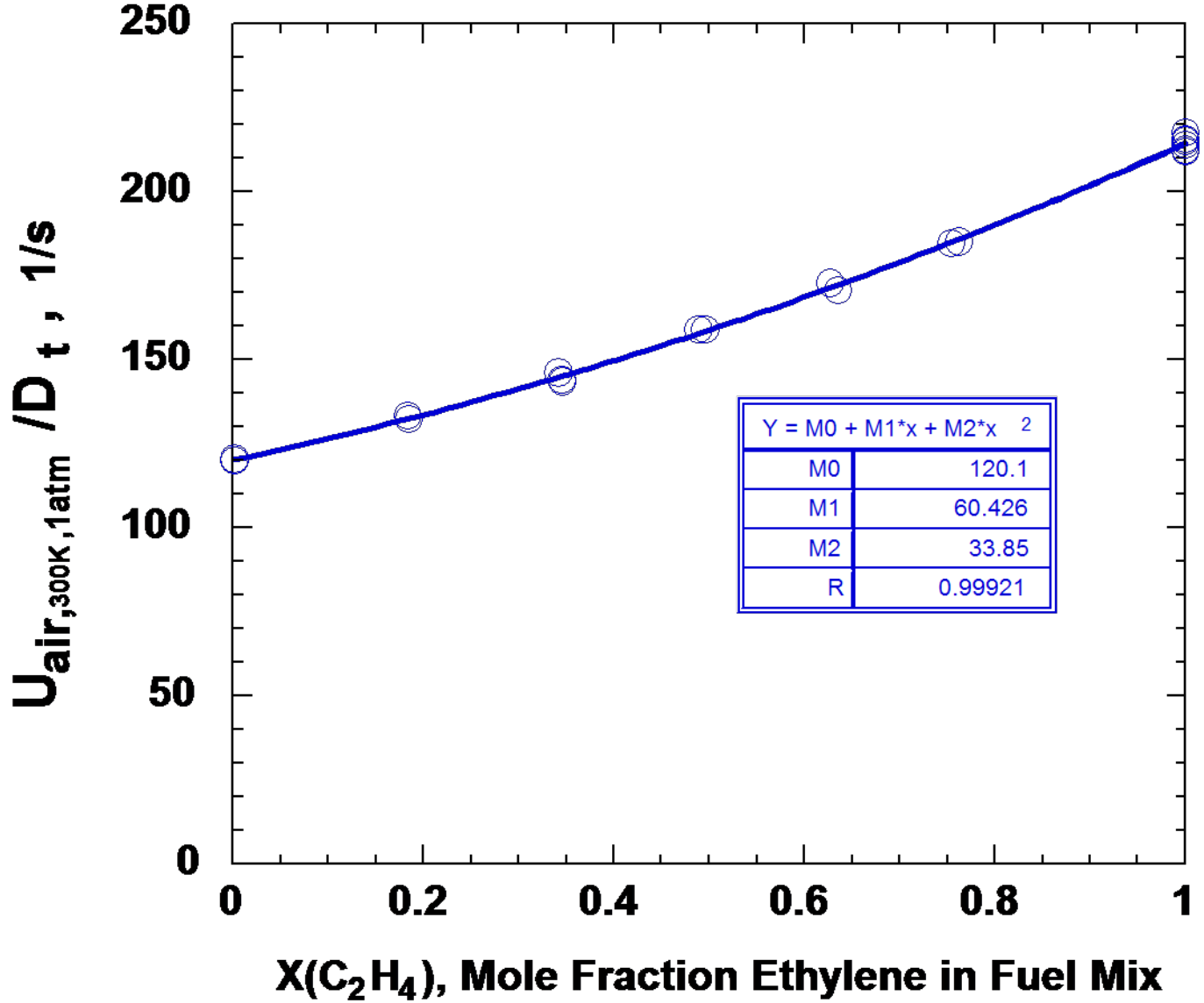
Effect of OJB Tube Diameter on Applied Stress Rate at Extinction, for Various Gaseous Hydrocarbon vs Air CFDFs



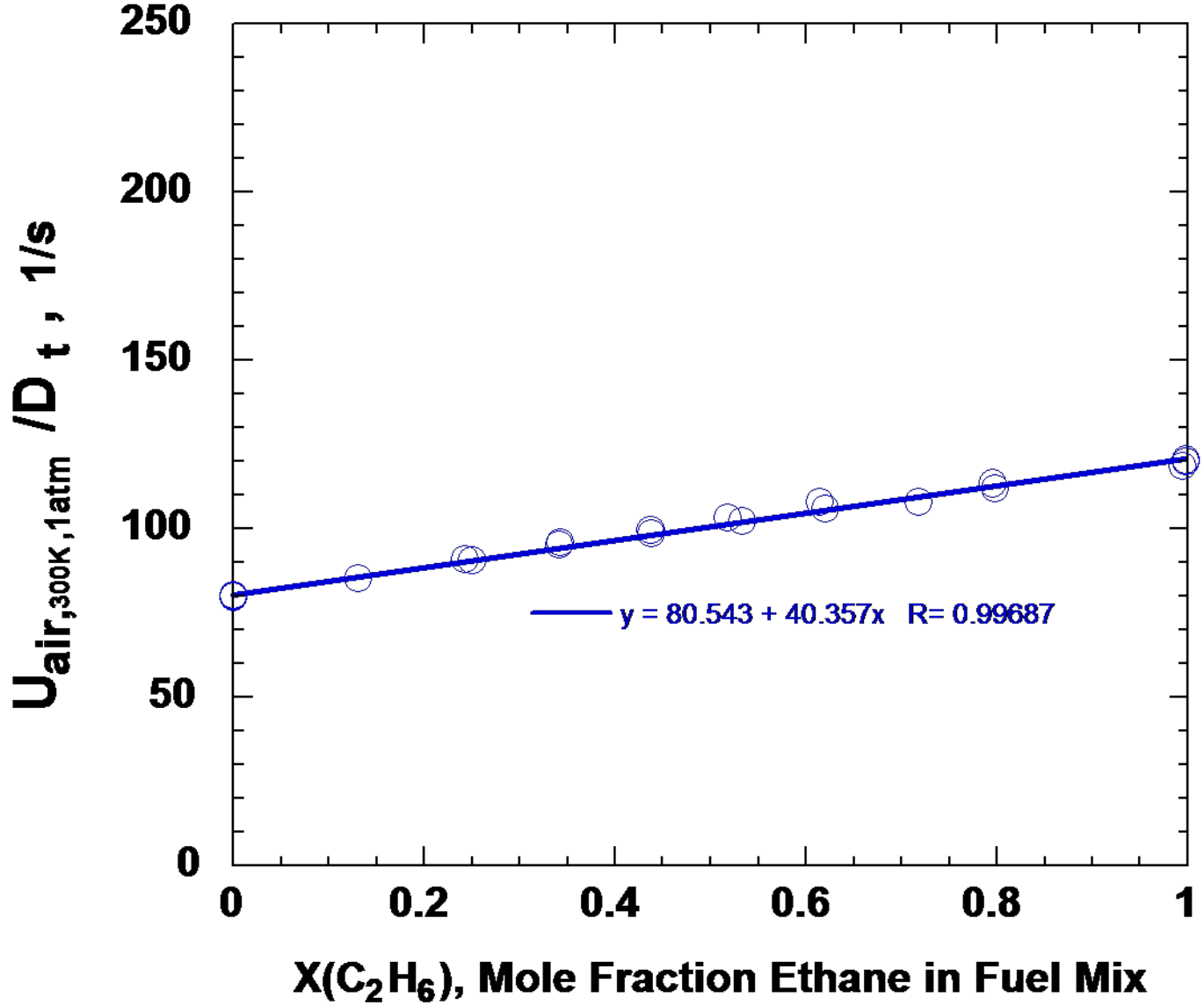
Applied Stress Rate at Extinction for Methane + Ethylene Fuel Mix vs Air Counterflow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



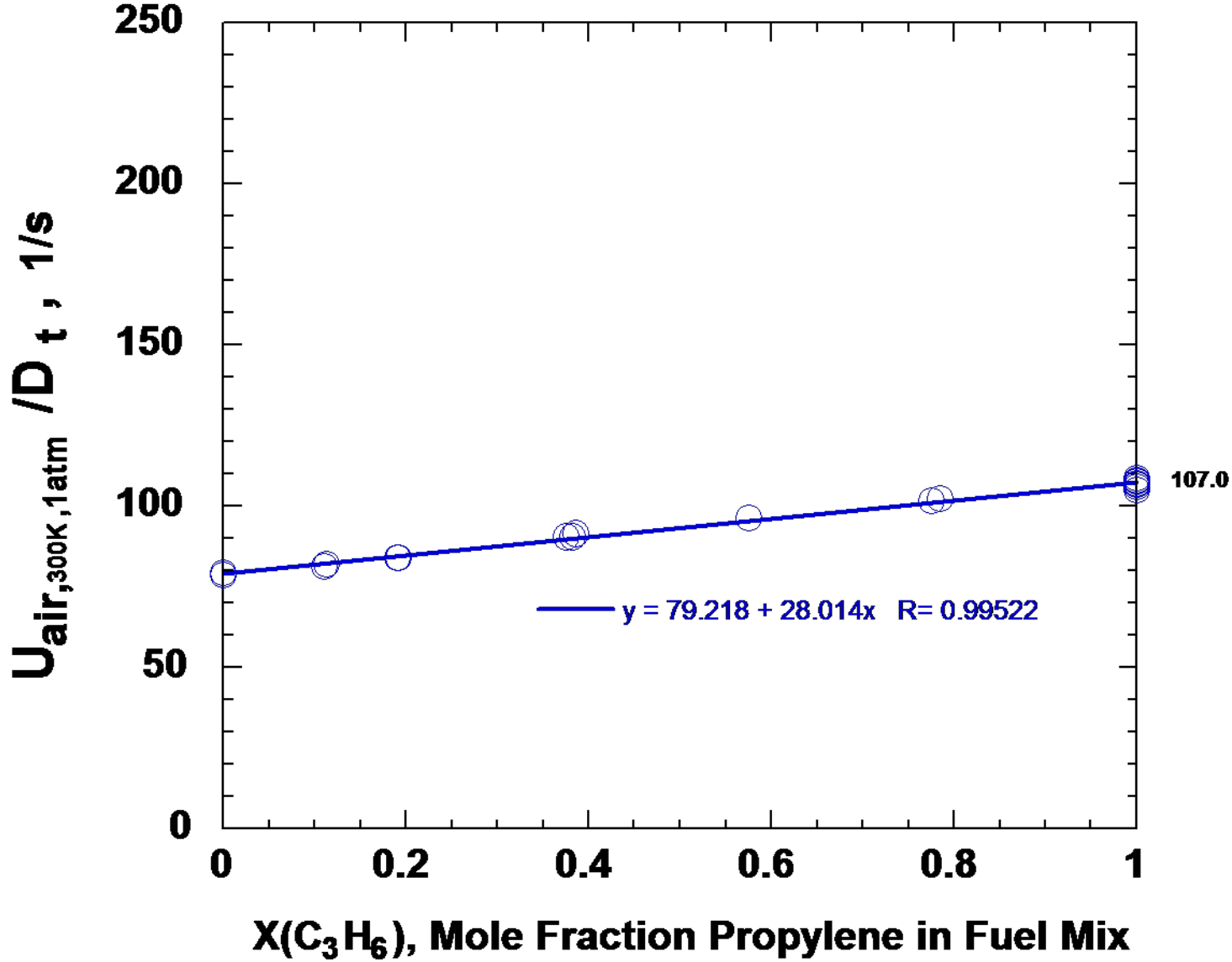
Applied Stress Rate at Extinction for Ethane + Ethylene Fuel Mix vs Air Counterflow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



Applied Stress Rate at Extinction for Methane + Ethane Fuel Mix vs Air Counterflow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



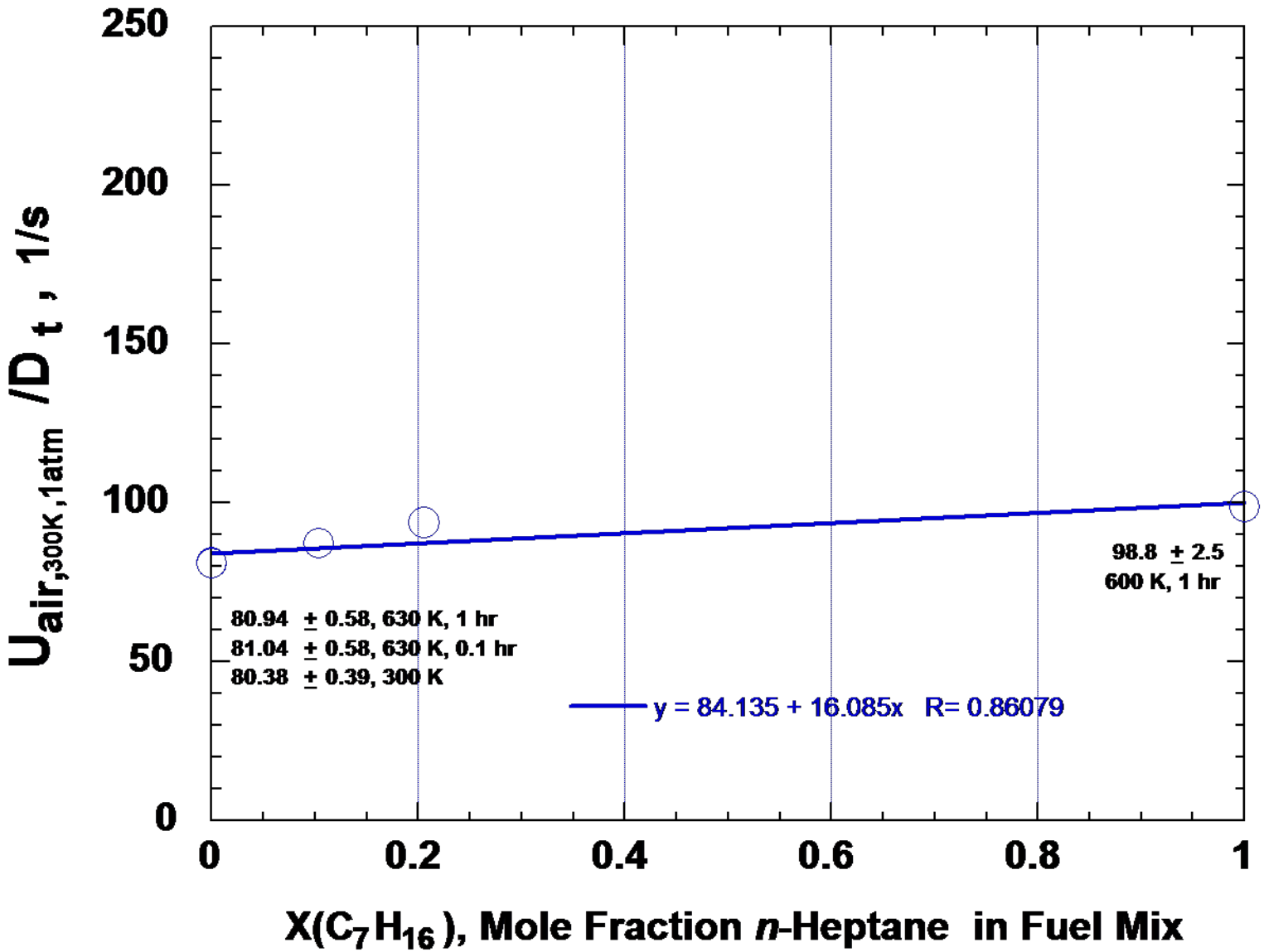
Applied Stress Rate at Extinction for Methane + Propylene Fuel Mix vs Air Counterflow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



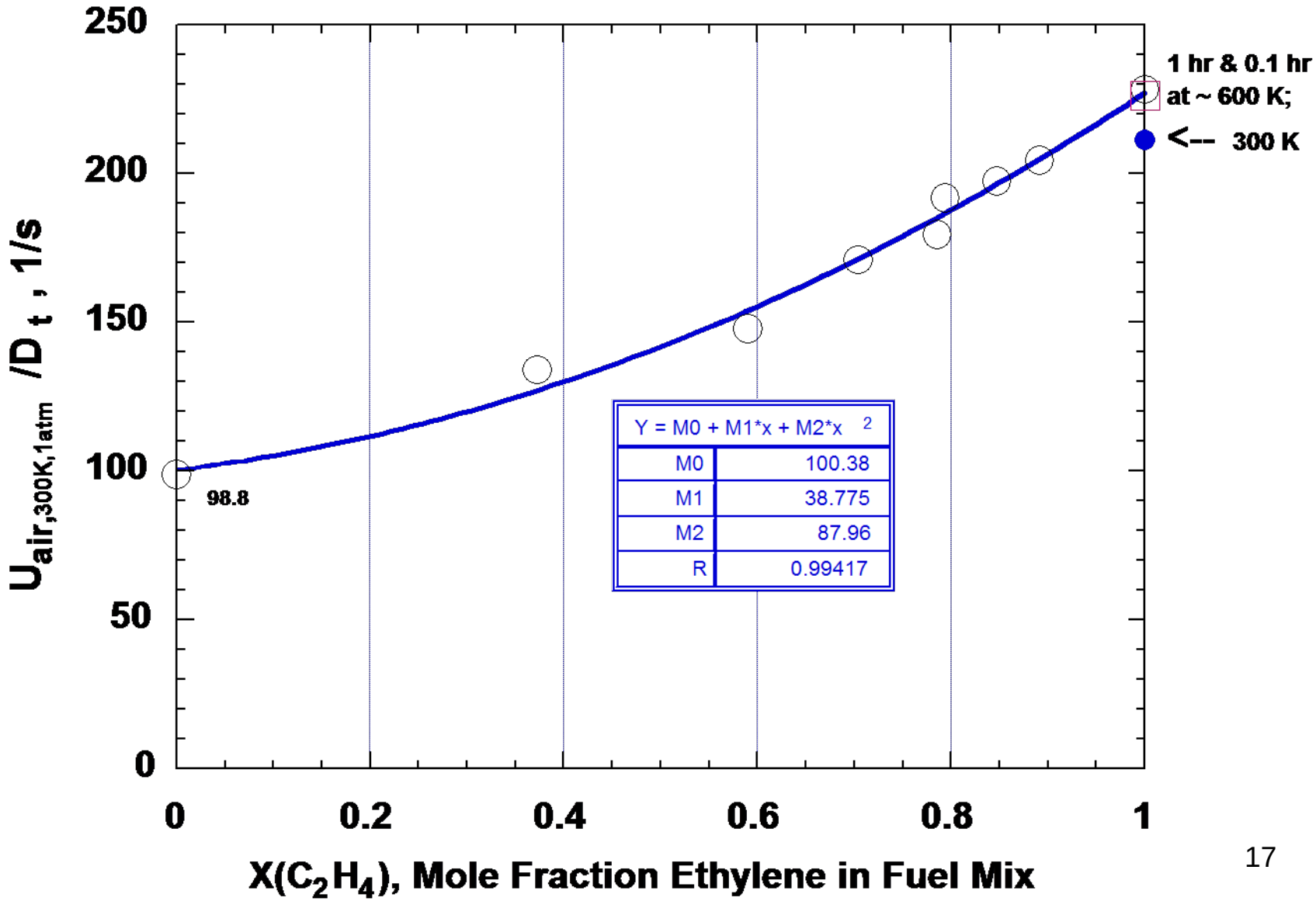
Definition of HIFiRE Gaseous Surrogate Fuel

- **Gaseous Binary Surrogate that Mimics Cracked JP-7 “like” Fuel**
  - Determine binary-mixture Flame Strength (FS) for a Counter Flow Diffusion Flame (CFDF), that equals FS for a ternary baseline surrogate mixture proposed by Colket & Spadaccini (JPP, 2001).
  - Ternary baseline surrogate (above) was based on extensive shock tube ignition (and cracking) data for methane, ethylene, and *n*-heptane (30/60/10 mole %), that mimics a cracked (reformed) JP-7 “like” fuel.
  - Gaseous 64/36 ethylene / methane surrogate mixture was derived from detailed OJB data (documented in AIAA 2007-5664; JANNAF-847, May, 2008; and JANNAF-752, Dec. 2009).

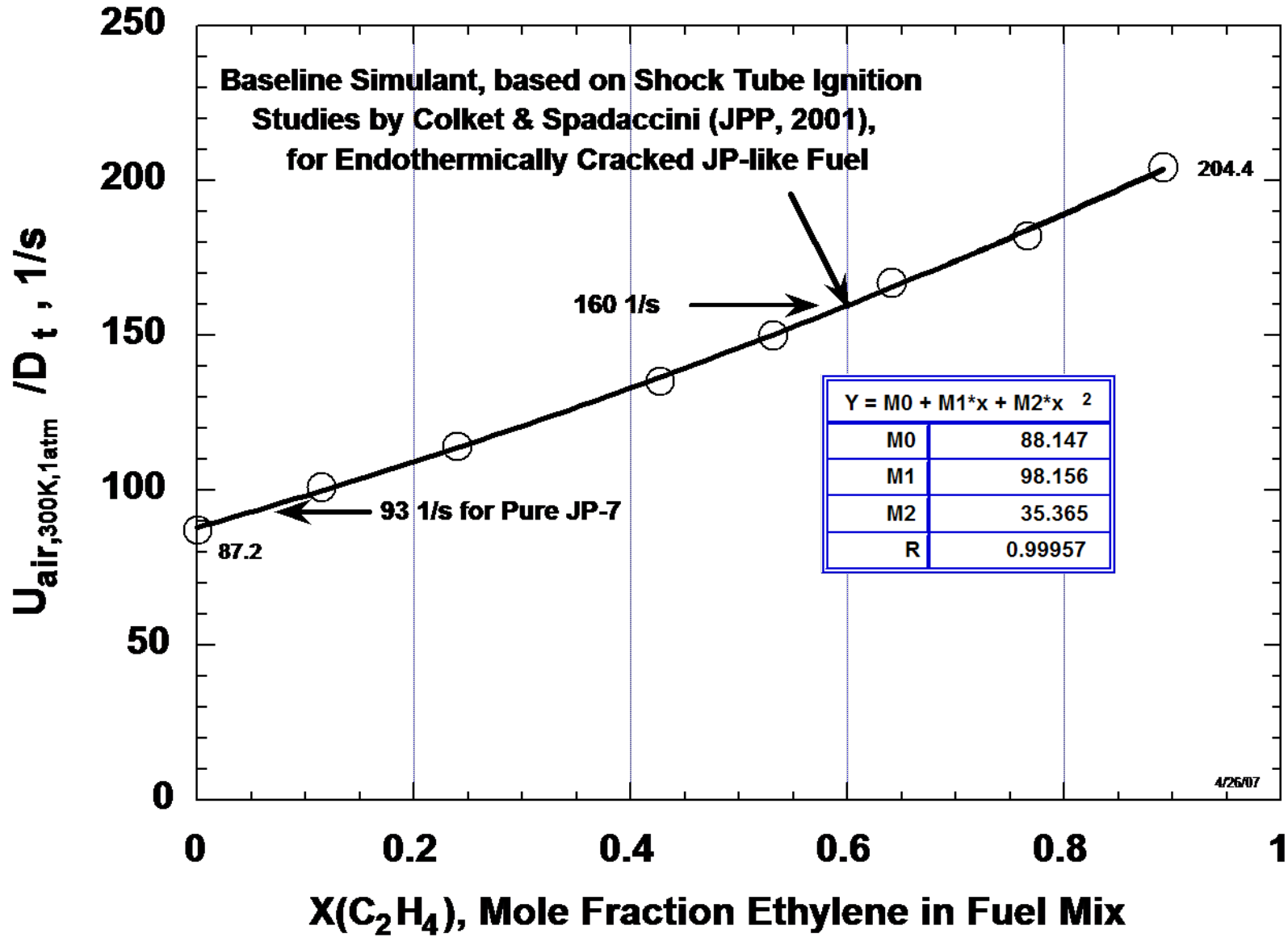
Applied Stress Rate at Extinction for 600 + K Methane + n-Heptane Fuel Mix vs Air Counterflow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



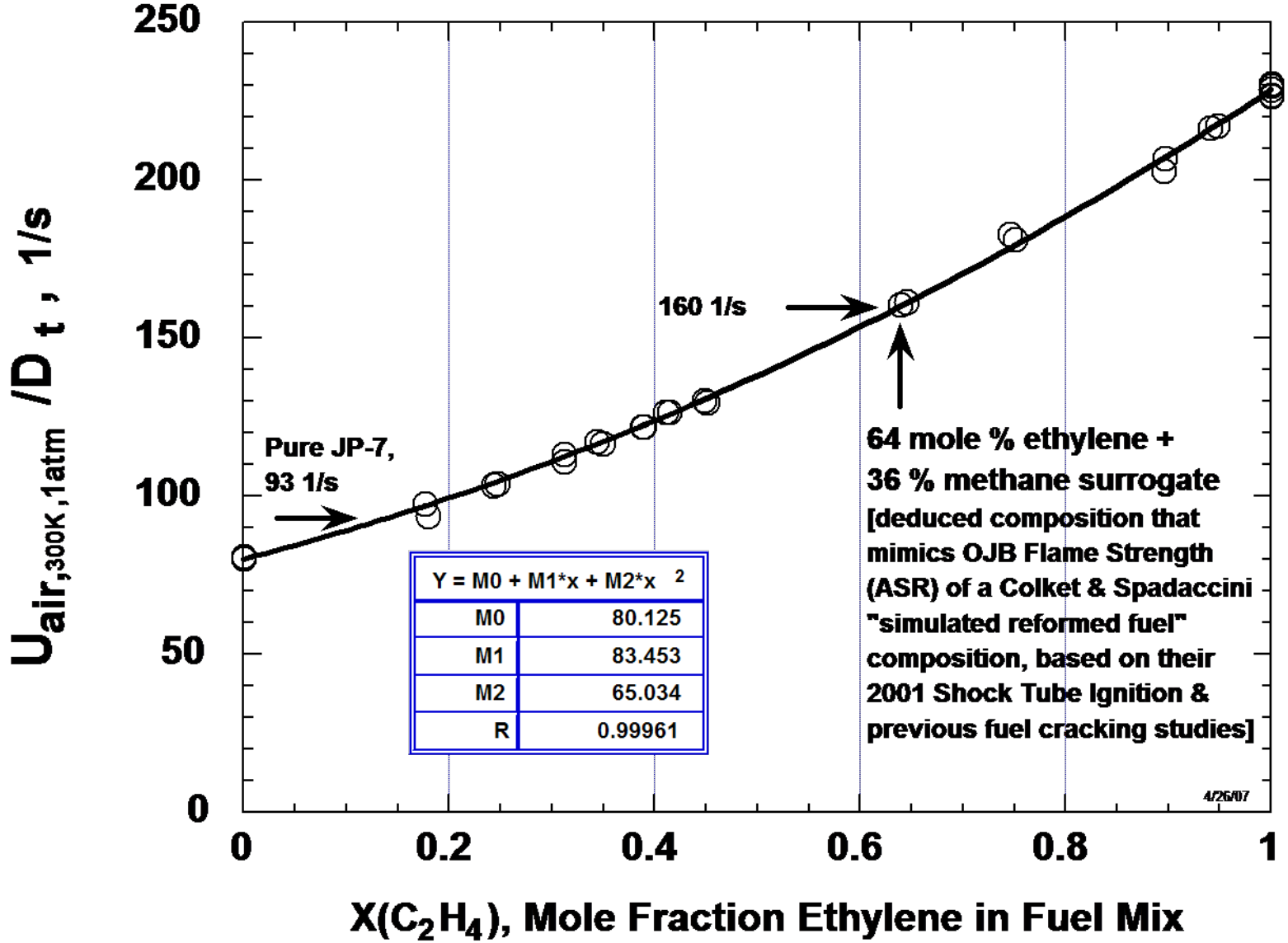
Applied Stress Rate at Extinction of Gaseous n-Heptane + Ethylene Fuel Mix vs Air Counter Flow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



Applied Stress Rate at Extinction of 600 K Methane + Ethylene +10.8 mole % gaseous *n*-Heptane Fuel vs Air Counter Flow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



Applied Stress Rate at Extinction for 600 K Methane + Ethylene Fuel Mixtures vs Air Counterflow Diffusion Flames, 7.56 mm Tube-OJB, 1 atm



$Y = M0 + M1*x + M2*x^2$	
M0	80.125
M1	83.453
M2	65.034
R	0.99961

Effects of O_2 (and NO) Concentration on Extinction Limits -- for "Idealized" HIFiRE Flameholding

✸ **Motivation:**

★ Test air contamination, from production of nitric oxide with consumption of O_2 in Arc-Jet-Heater Facility, occurs in tests of HIFiRE scramjet combustors.

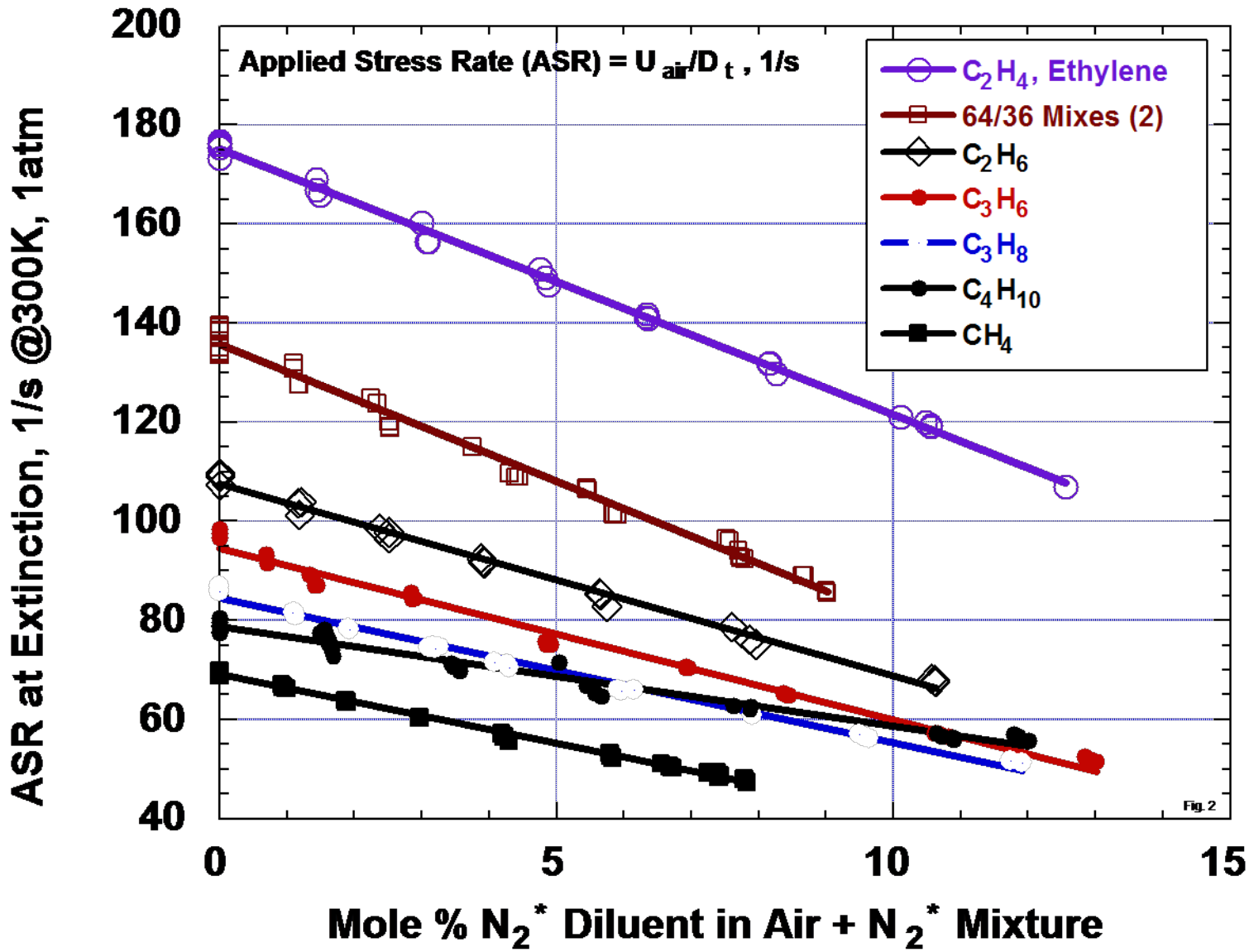
★ Flight testing of the HIFiRE vehicle may experience an offset in robust flameholding, mode transition, and/or flameout, due to the "final" switch from facility contaminated air to clean air.

★ Development of advanced HC-fueled scramjets will require <u>greatly improved</u> chemical kinetics for accurate simulations of flameholding during flight in clean and facility-contaminated air.

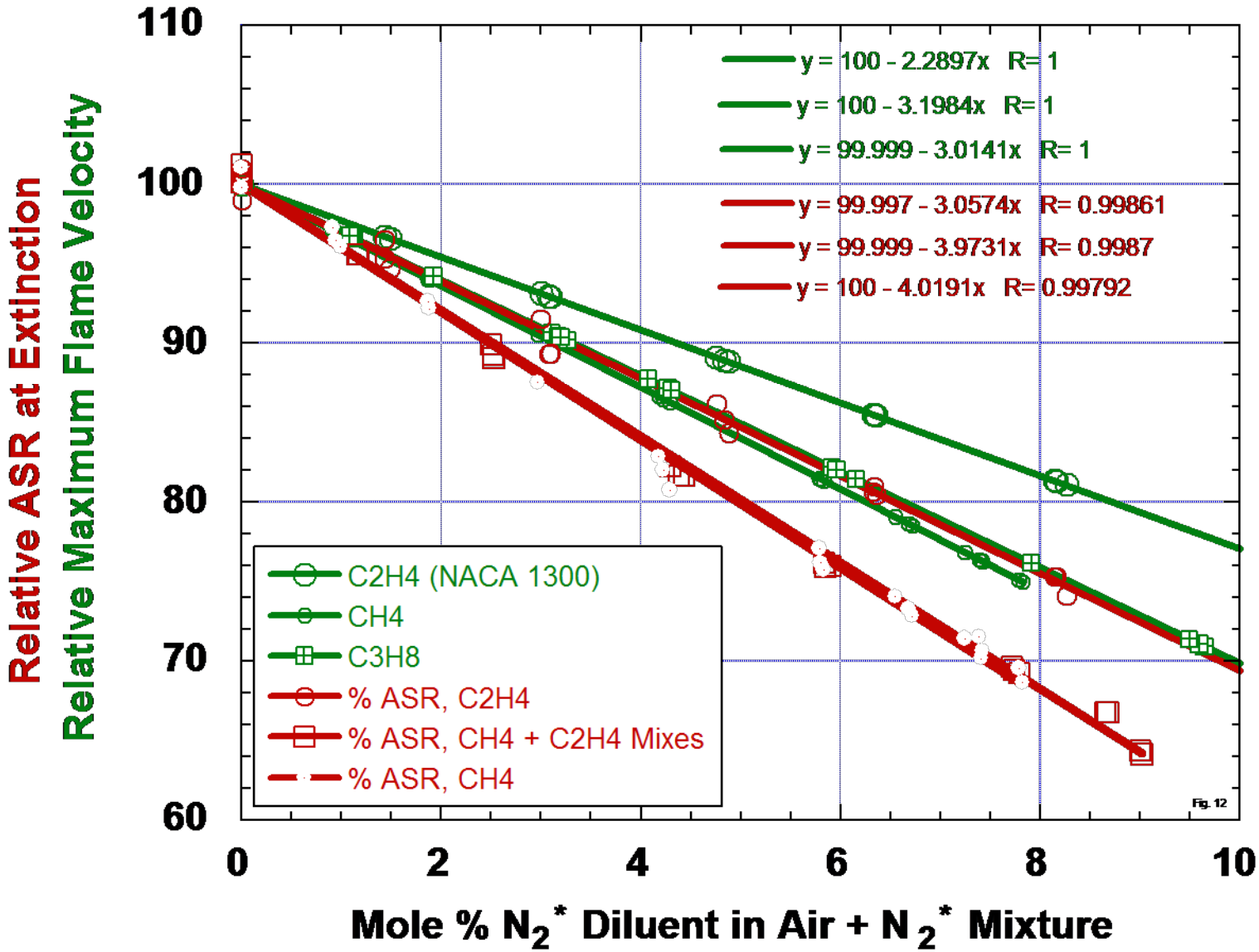
✸ **Related Work:**

★ Compared with our earlier OJB extinction results (JANNAF-847, May, 2008), 1-D simulations (UVa) of ethylene vs. air flame extinction were high by ~ 45 %, based on USC (2007) kinetics.

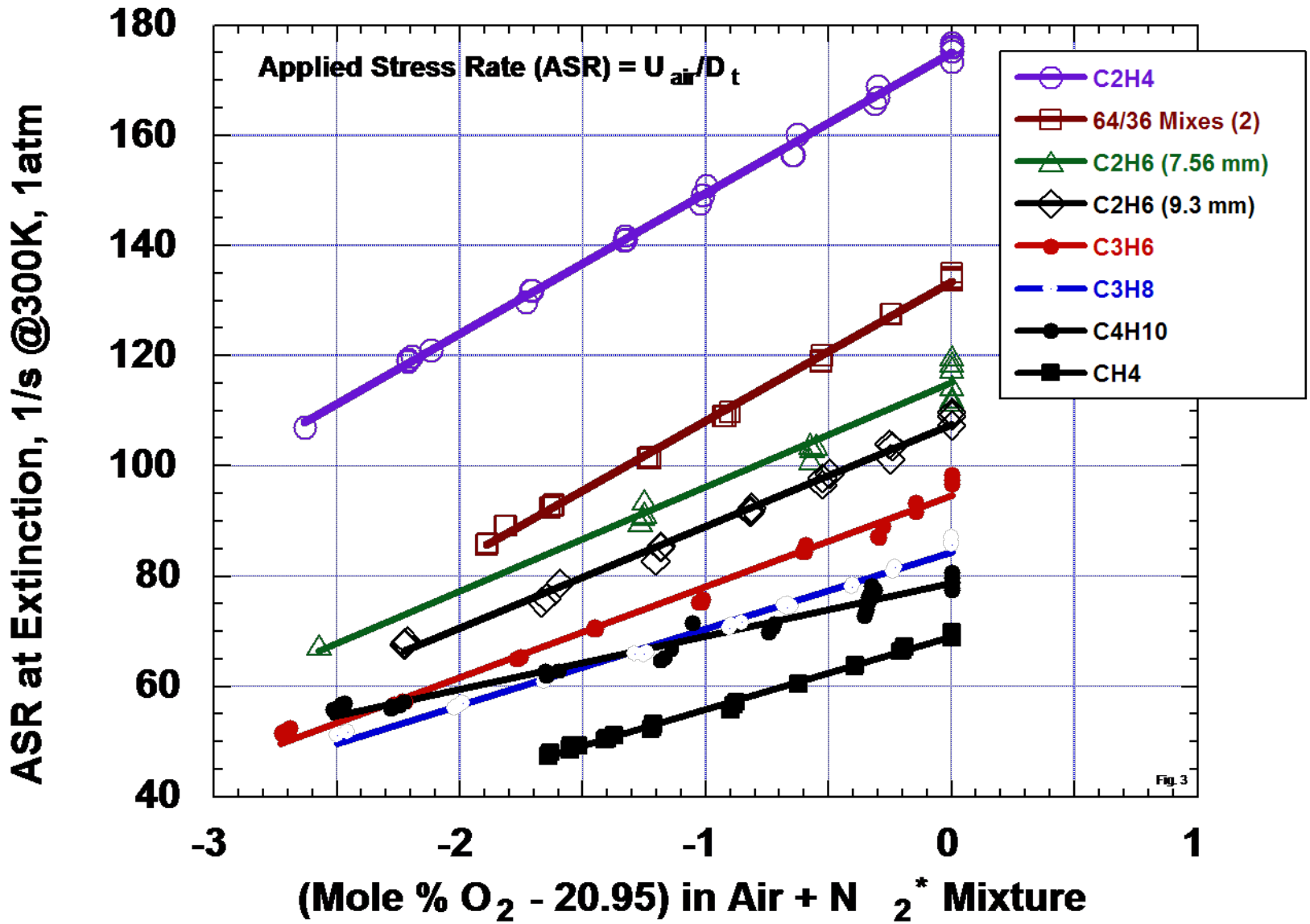
Effects of N_2^* Dilution of Air on Extinction of HC vs. Air CFDFs, using 9.3 mm Tube-OJB System at 1 atm



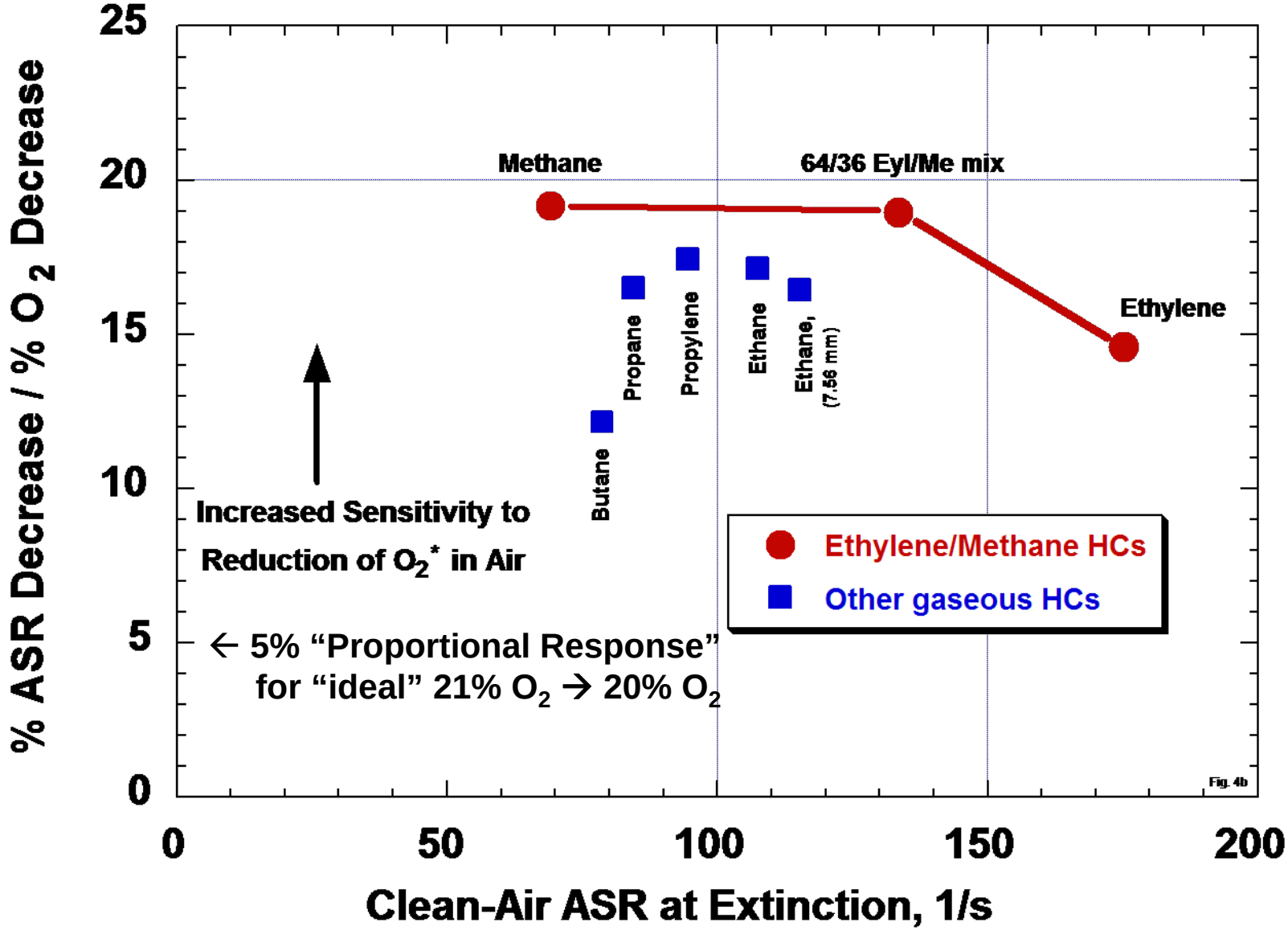
Effects of N_2 Dilution of Air on Extinction of HC vs. Air CFDFs, using 9.3 mm Tube-OJB Systems at 1 atm; and Comparison with Relative Maximum Flame Velocity [NACA Rpt. 1300, (1959)]



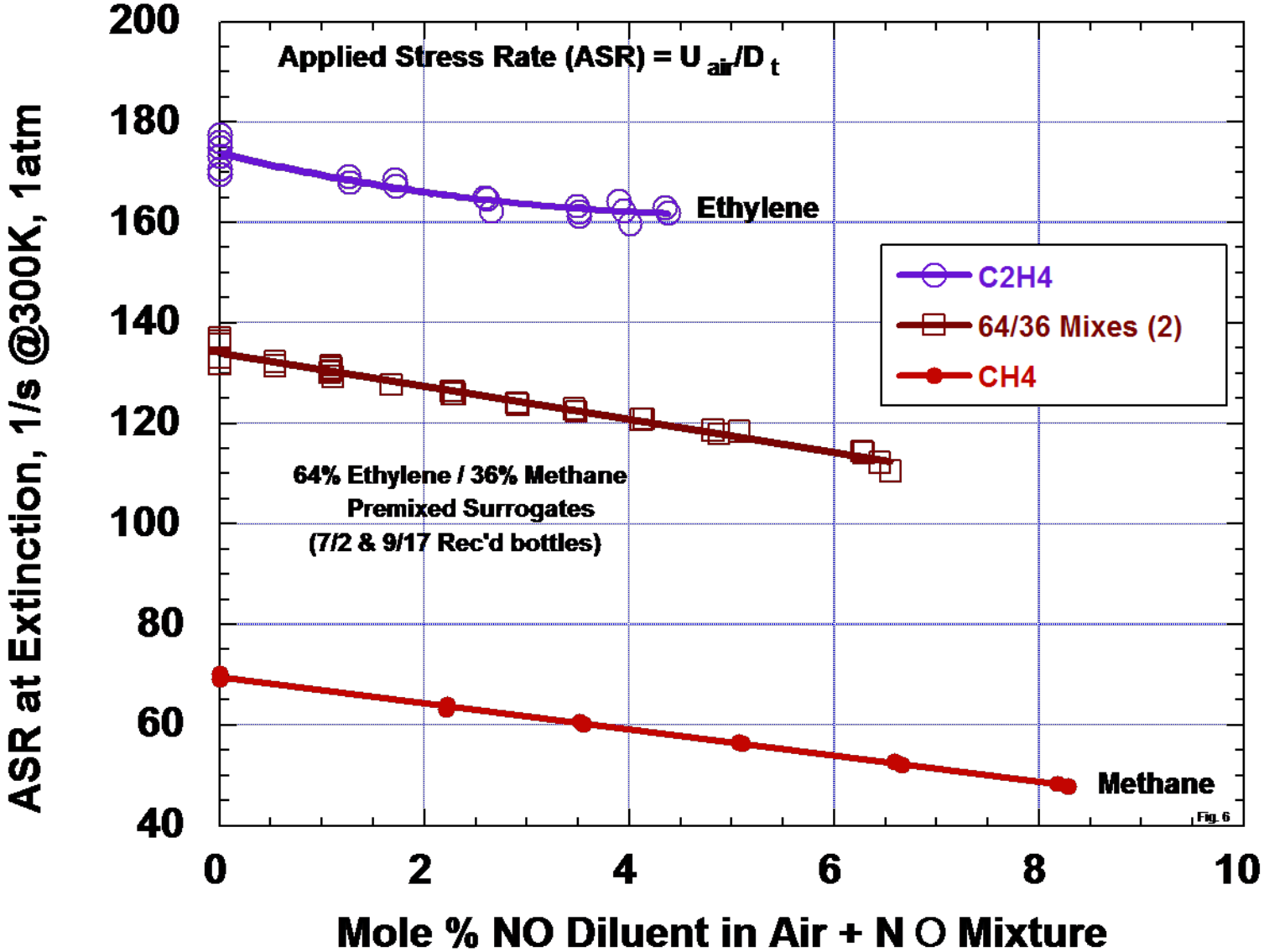
Effects of Mole % O_2 in Air on Extinction of HC vs. Air CFDFs, using 9.3 mm (and 7.56 mm for C_2H_6) Tube-OJB System at 1 atm



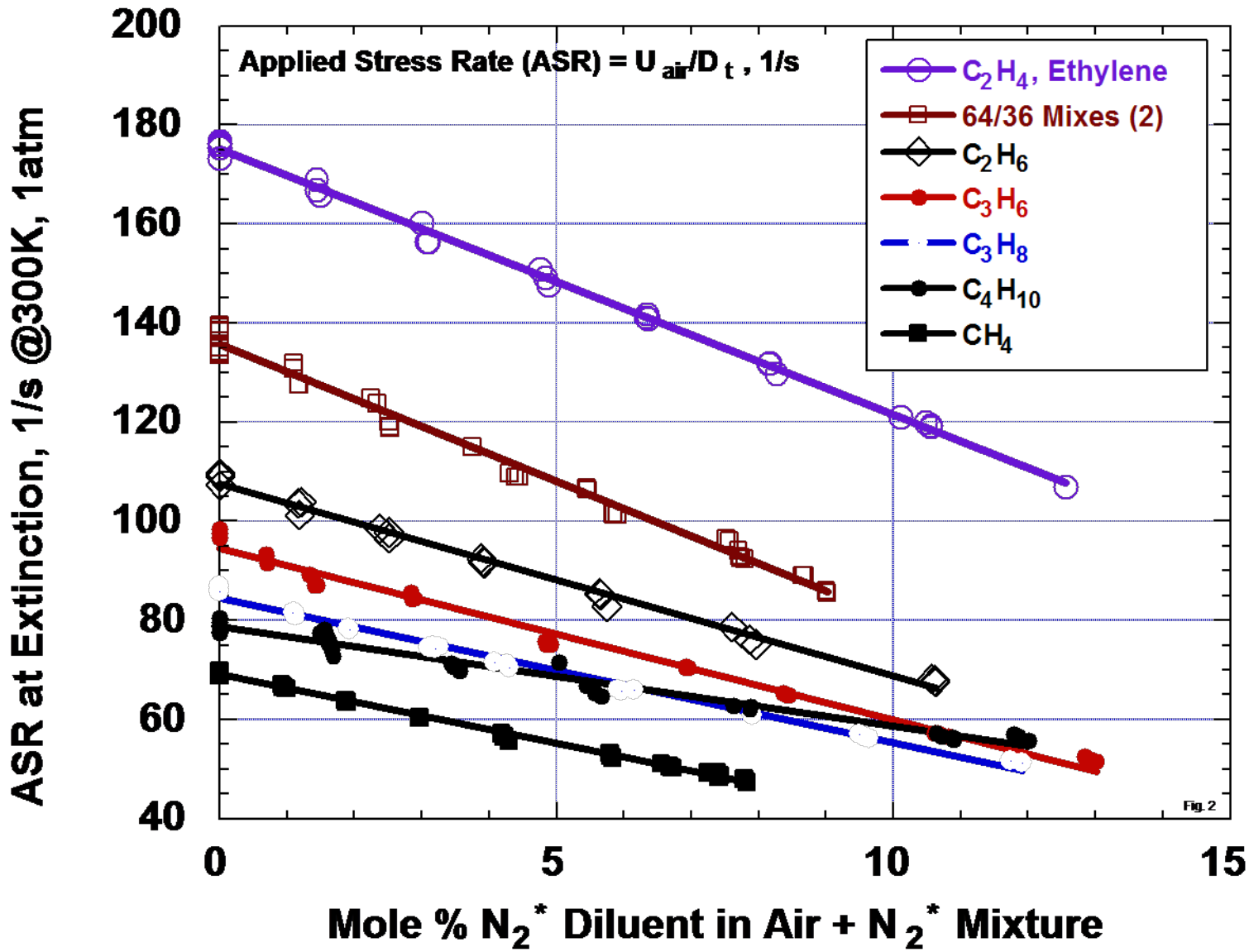
Sensitivity of ASR at Extinction due to Decreased O_2 in Air, for Various HCs vs. N_2^*–Contaminated Air, using 9.3 mm Tube-OJB System at 1 atm



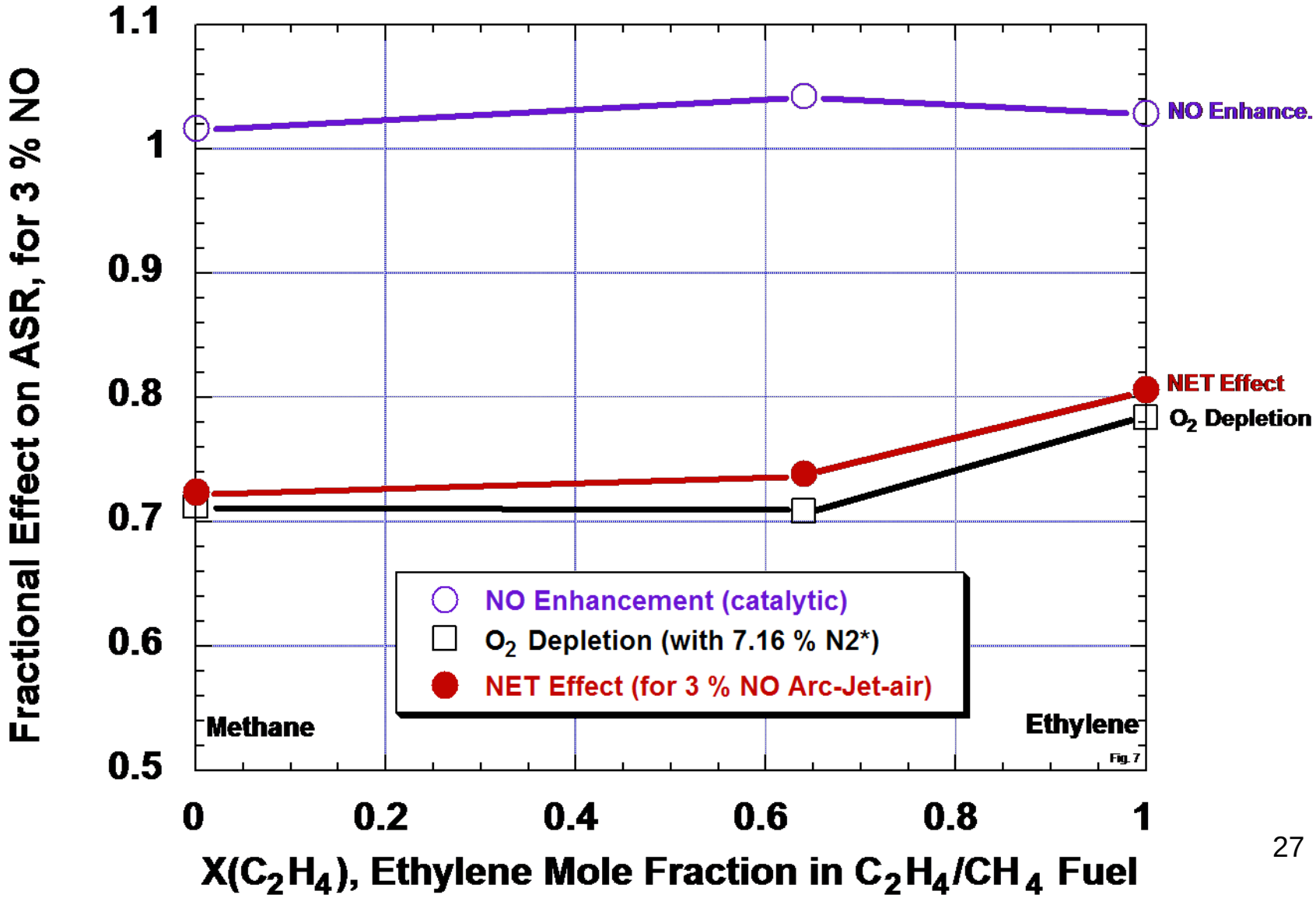
Effects of NO Dilution of Air on Extinction of HCs vs. Air CFDFs, using 9.3 mm Tube-OJB System at 1 atm



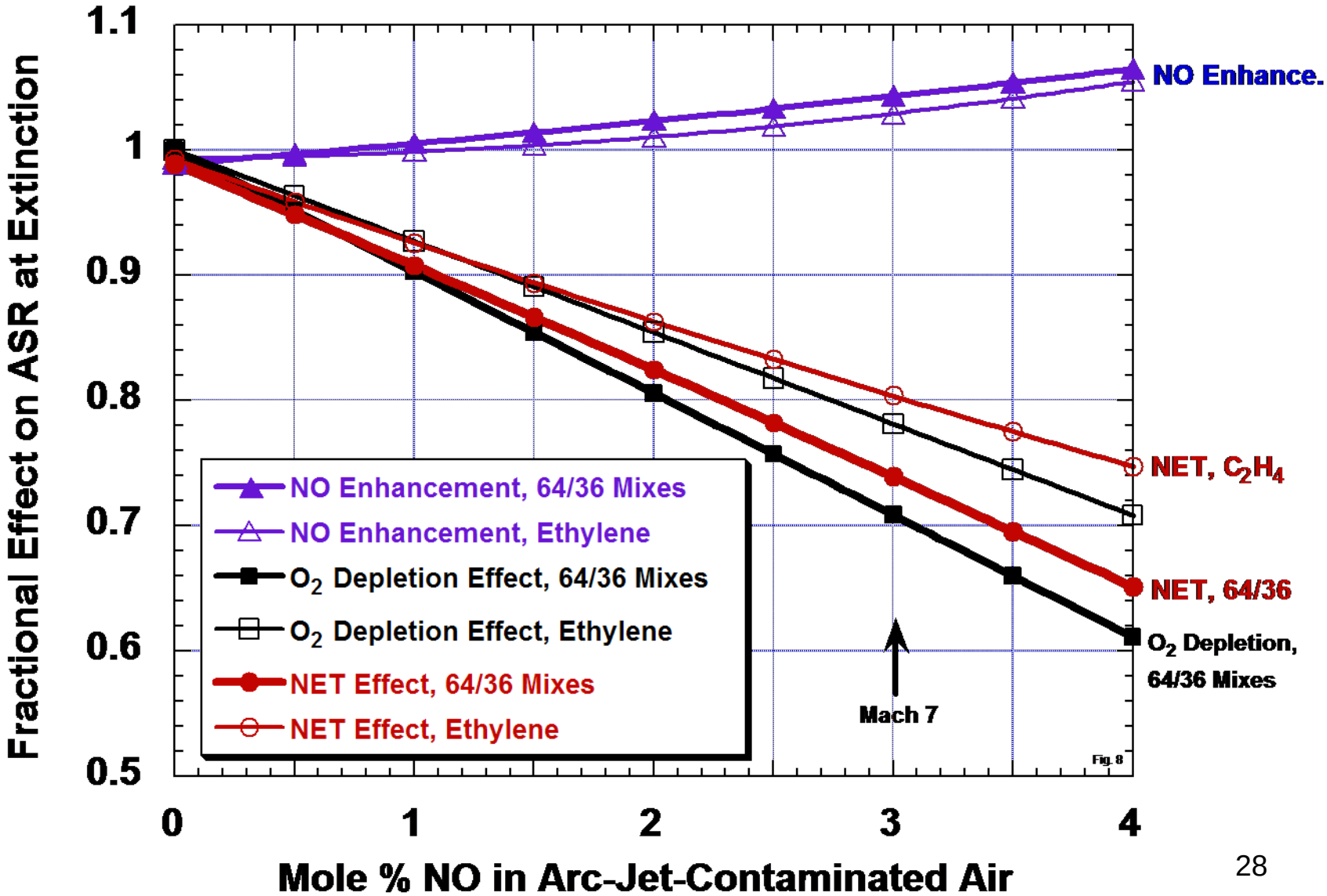
Effects of N_2^* Dilution of Air on Extinction of HC vs. Air CFDFs, using 9.3 mm Tube-OJB System at 1 atm



Fractional Effects on ASR at Extinction, for HC vs. Arc-Jet-Contaminated Air with 3 mole % NO: For NO Enhancement, Oxygen Depletion, and Net Effects on ASR, based on 9.3 mm Tube OJB at 1 atm.



Fractional Effects on ASR at Extinction, for Ethylene and 64/36 C_2H_4/CH_4 Surrogate Fuels vs. Arc-Jet-Contaminated Air: For "NO Enhancement", "Oxygen Depletion" and "Net" Effects, from 9.3 mm Tube OJB at 1 atm.



Re: Air Contamination Effects on "Ideal" Flameholding

- Very significant "oxygen-deficiency" weakening effects on flame extinction for all seven HCs tested. **Effects are ~ 2.5 times that for H_2.**

- "Nitric oxide (NO) enhancement" effects on flame extinction are small (to ~ 4 %) for methane, ethylene, the "64/36" mix, and probably most simple gaseous HCs.

- Because "oxygen-deficiency" weakening effects grow large (*and* ~ 2.5 times that for H_2), renewed scrutiny is needed for tests that alter local O_2 (e.g., vitiated air with O_2 make-up, and arc-heaters that consume O_2 to produce NO).

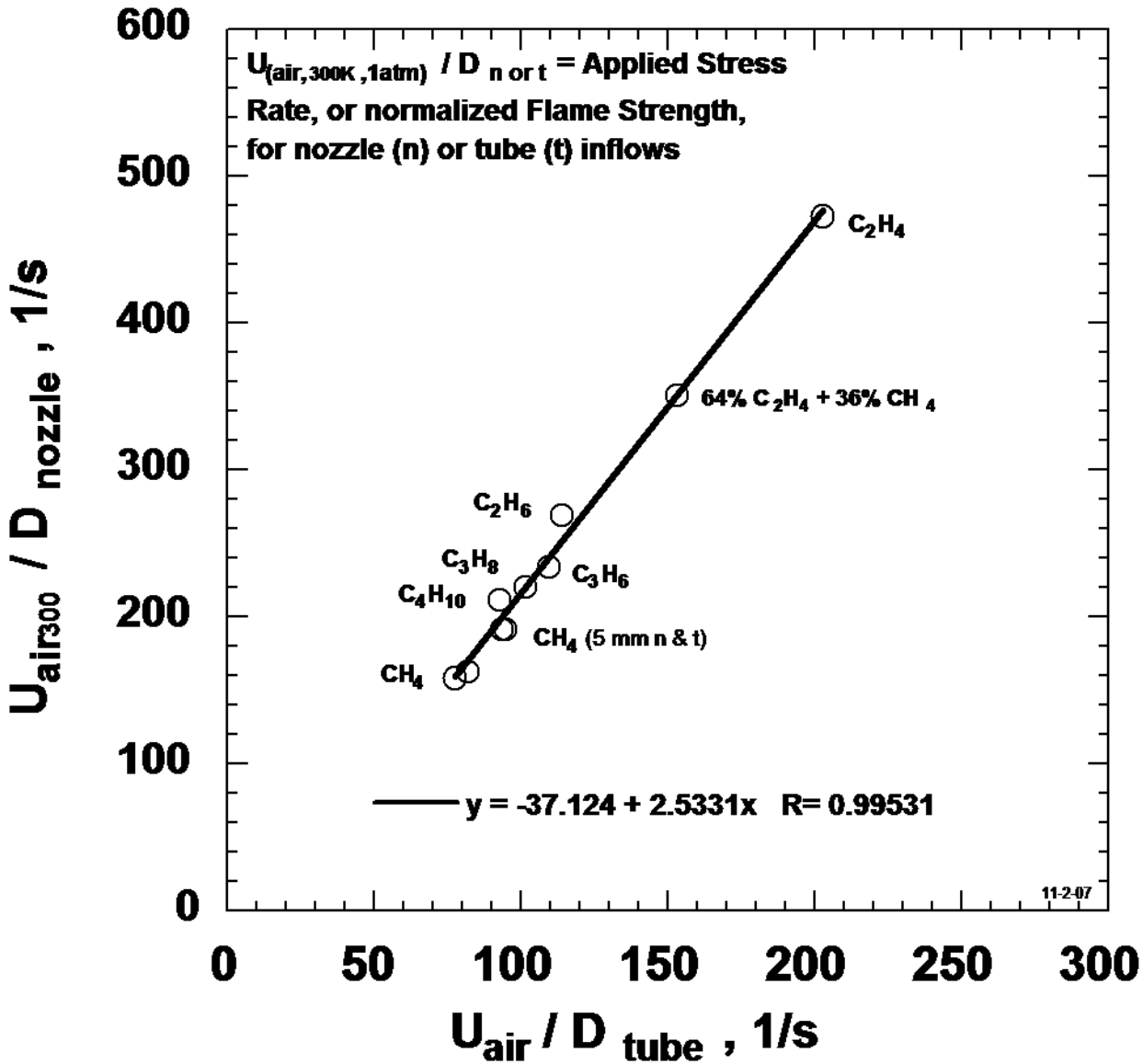
- The deduced 26 % reduction in FS for the "64/36" surrogate fuel vs. Arc-Jet-contaminated air with 3 % NO suggests that "clean air" flameholding processes *may be strengthened* during flight.

(1) Extinction Limits for 7 Gaseous HCs, from Convergent-Nozzle and Uniform-Tube OJBs;

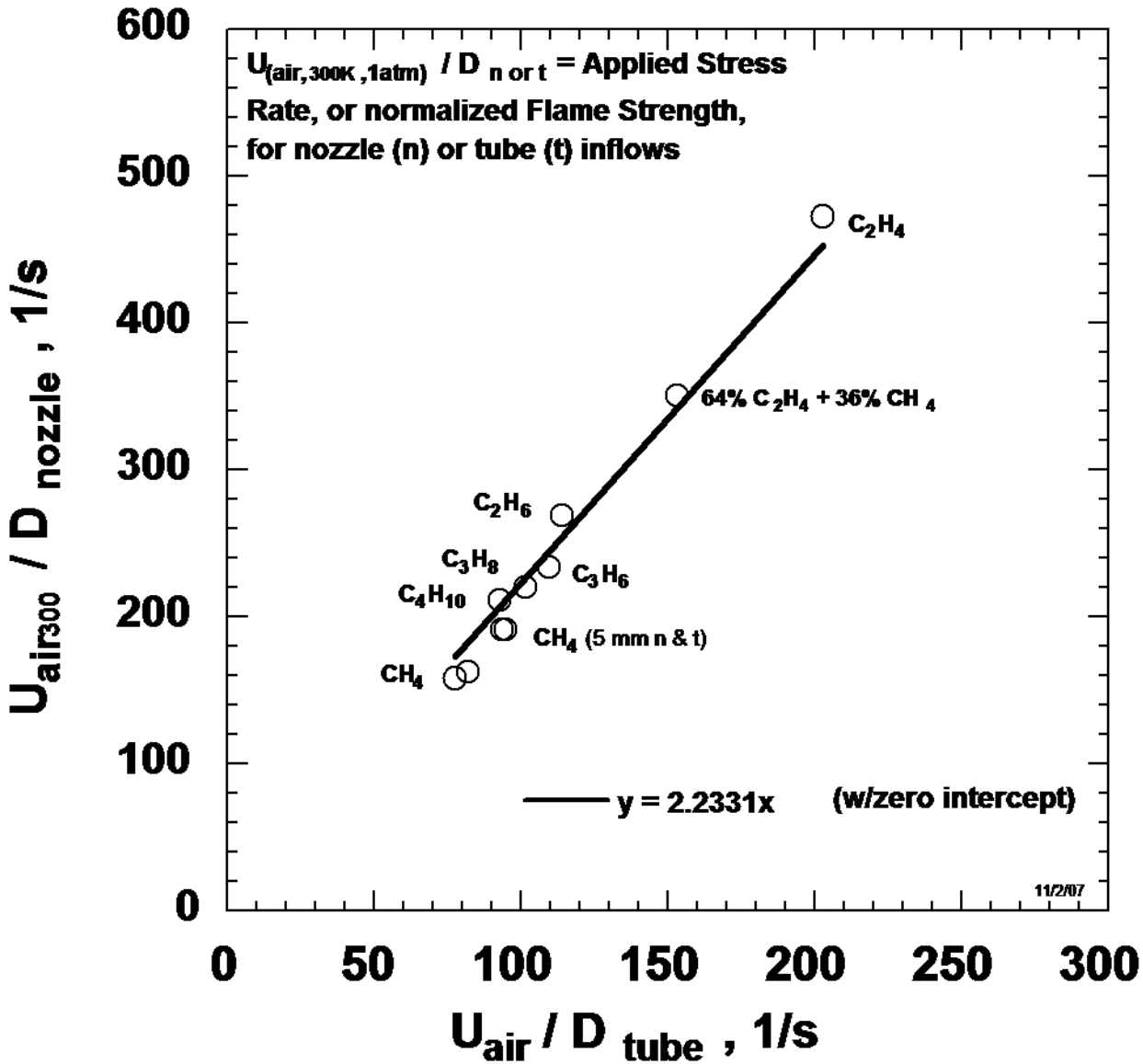
(2) Transformation of Global Strain Rates to "Absolute" Input Axial Strain Rate Scales;

(3) Comparisons with Published Results.

Extinction-Limit "Idealized Flameholding Scale," from 7.2 mm Convergent Nozzle- and 7.5 mm Straight Tube-OJBs, for gaseous HCs vs Air CFDFs, using Best Linear Fit WITH INTERCEPT



Extinction-Limit "Idealized Flameholding Scale," from 7.2 mm Convergent Nozzle- and 7.5 mm Straight Tube-OJBs, for gaseous HCs vs Air CFDFs, using Linear Fit WITH ZERO INTERCEPT



Comparison of Rolon's LDA-Measured Strain Rates for Variable Separation of 25 mm Contoured Nozzles, Air vs Air. Rolon et. al, Exp. in Fluids, 11, 313-324 (1991)

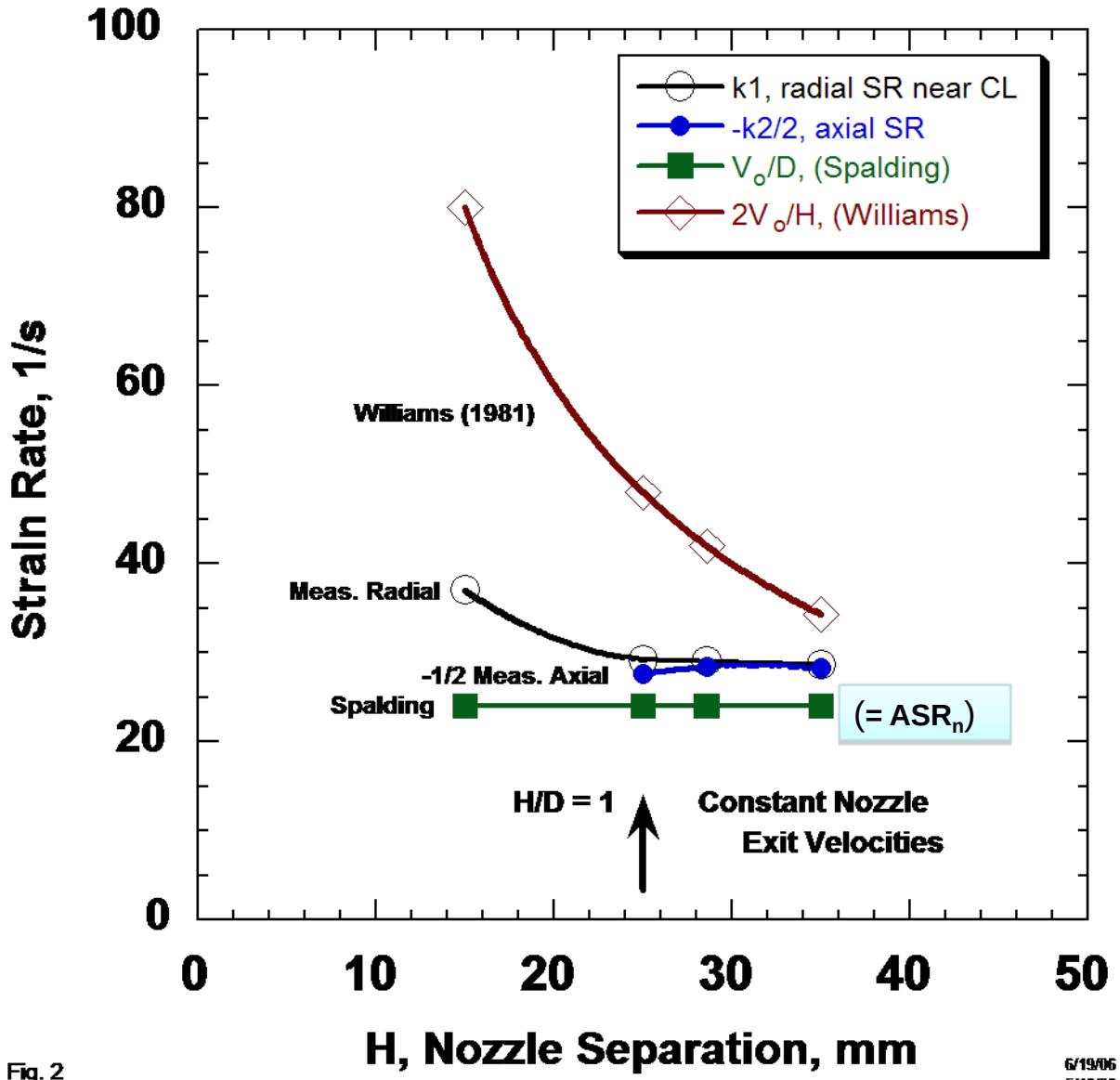
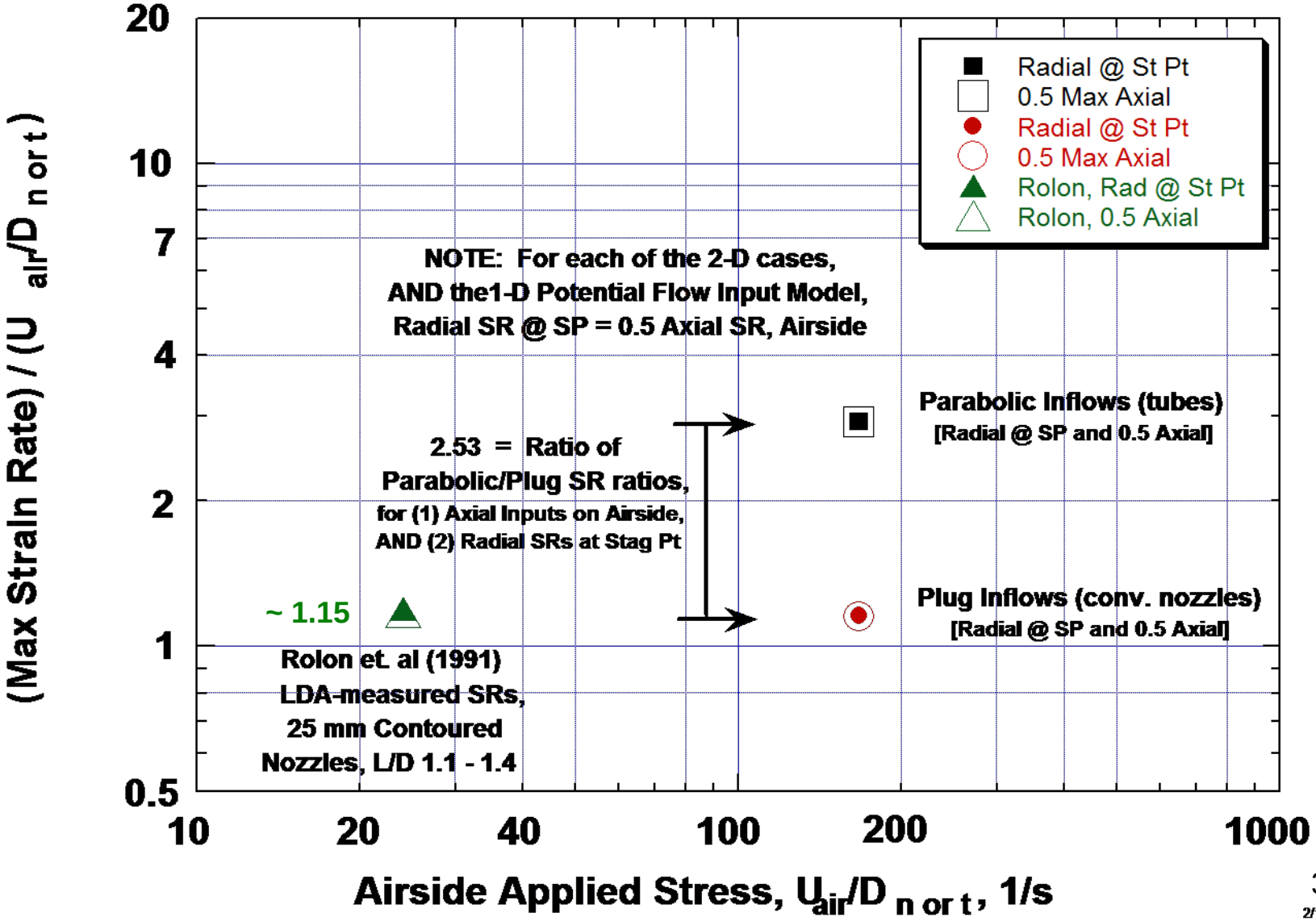


Fig. 2

6/19/06
5/16/06

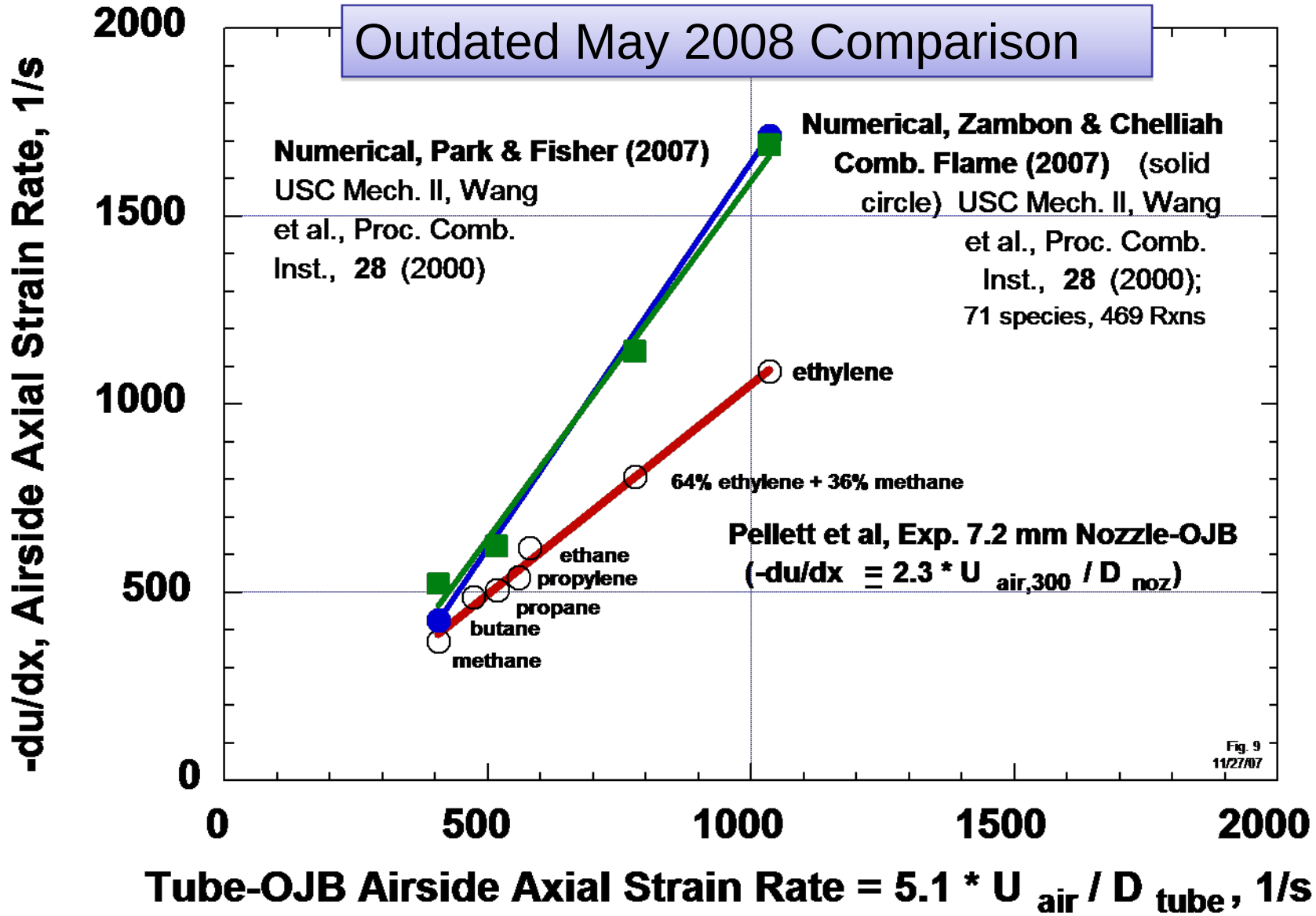
2-D Numerical Strain Rate Ratios for Cold Opposed Jet Air Flows, using 3 mm OJB's, 6 mm spacing, and both Plug and Parabolic Inflow Profiles

[2-D Results from Dissertation by Kyu C. Hwang, Old Dominion University, May 2003]

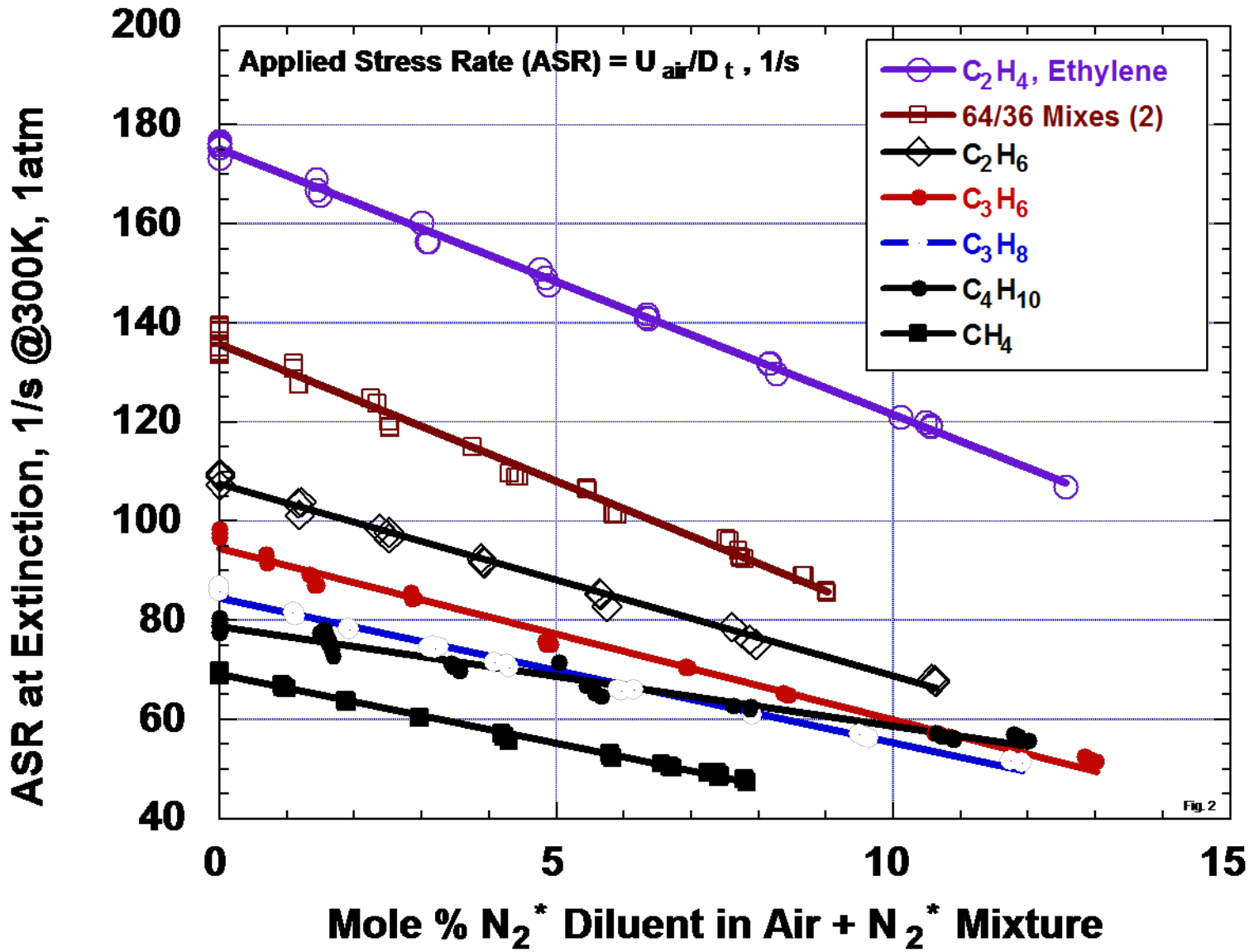


2/17/06
2/2/06

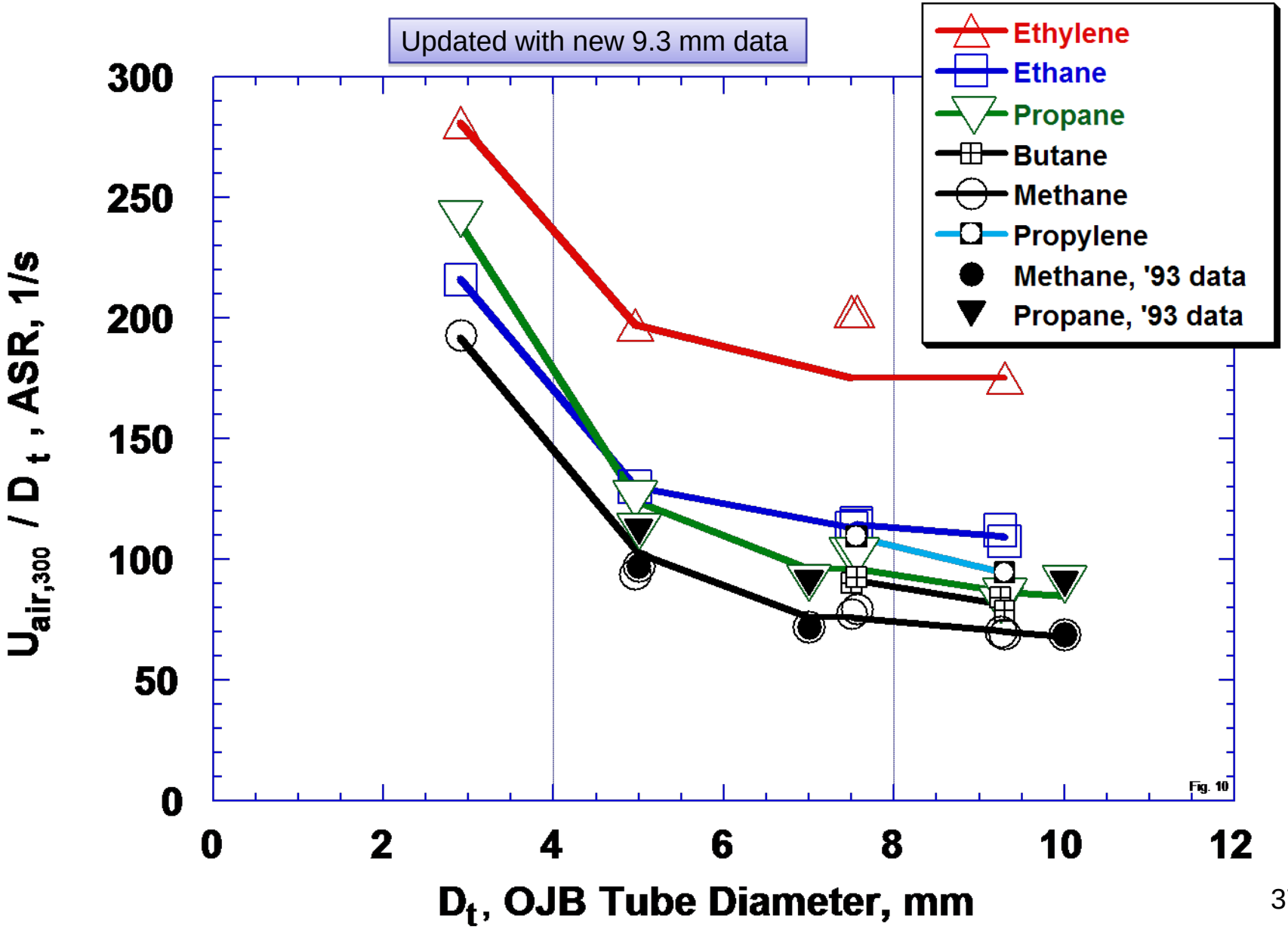
Comparison of Experimental and Numerical Strain-Induced Extinction Limits for Fuel vs Air Counterflow Diffusion Flames at 1 atm, Using Best Estimates of Airside Axial Strain Rate



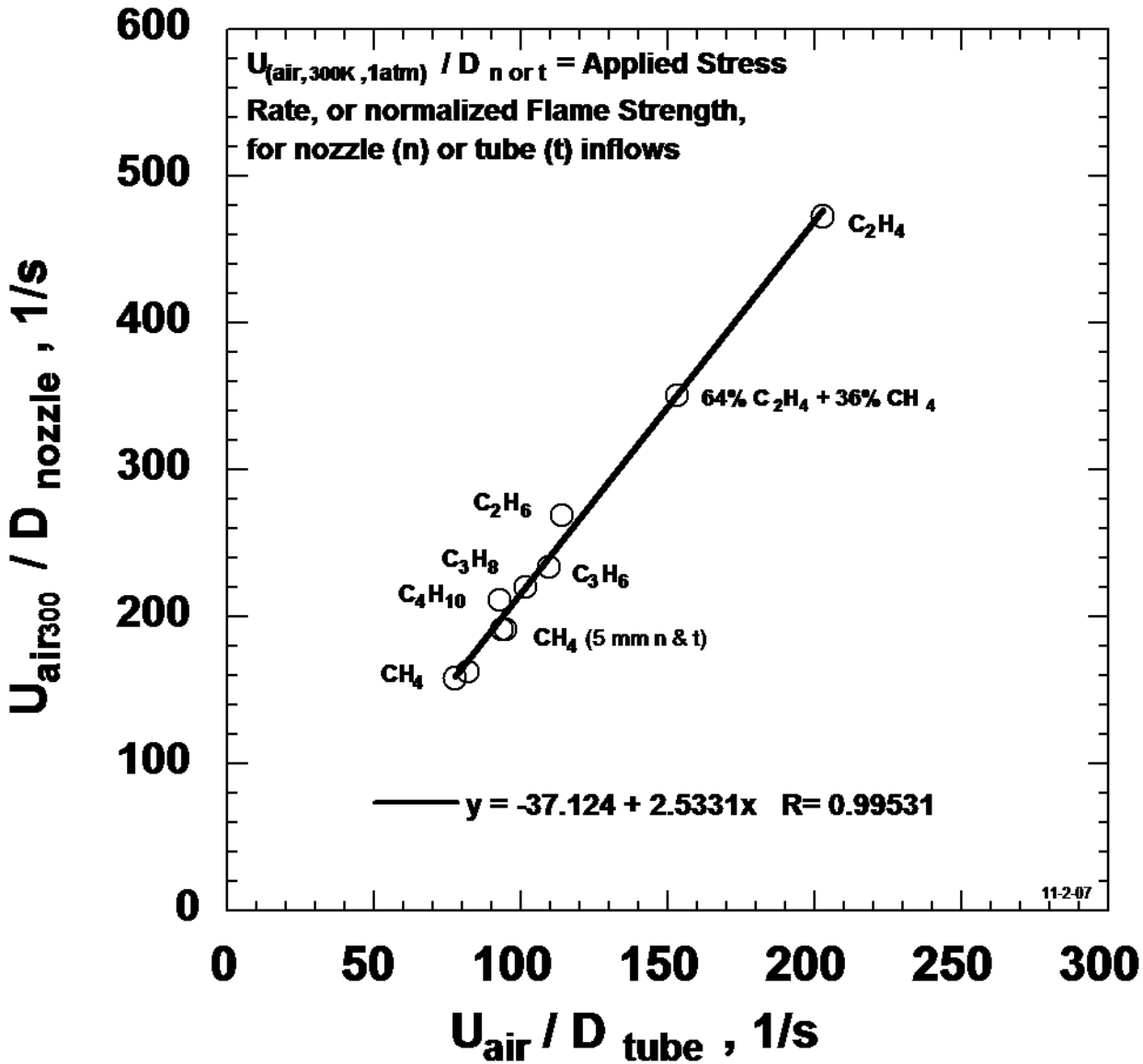
Effects of N_2^* Dilution of Air on Extinction of HC vs. Air CFDFs, using 9.3 mm Tube-OJB System at 1 atm



Effect of OJB Tube Diameter on Applied Stress Rate at Extinction, for Various Gaseous Hydrocarbon vs Air CFDFs



Extinction-Limit "Idealized Flameholding Scale," from 7.2 mm Convergent Nozzle- and 7.5 mm Straight Tube-OJBs, for gaseous HCs vs Air CFDFs, using Best Linear Fit WITH INTERCEPT



Transformation of Extinction ASR's from Tube-OJB to Best Estimates of Airside Axial Strain Rate for Convergent Nozzle-OJB

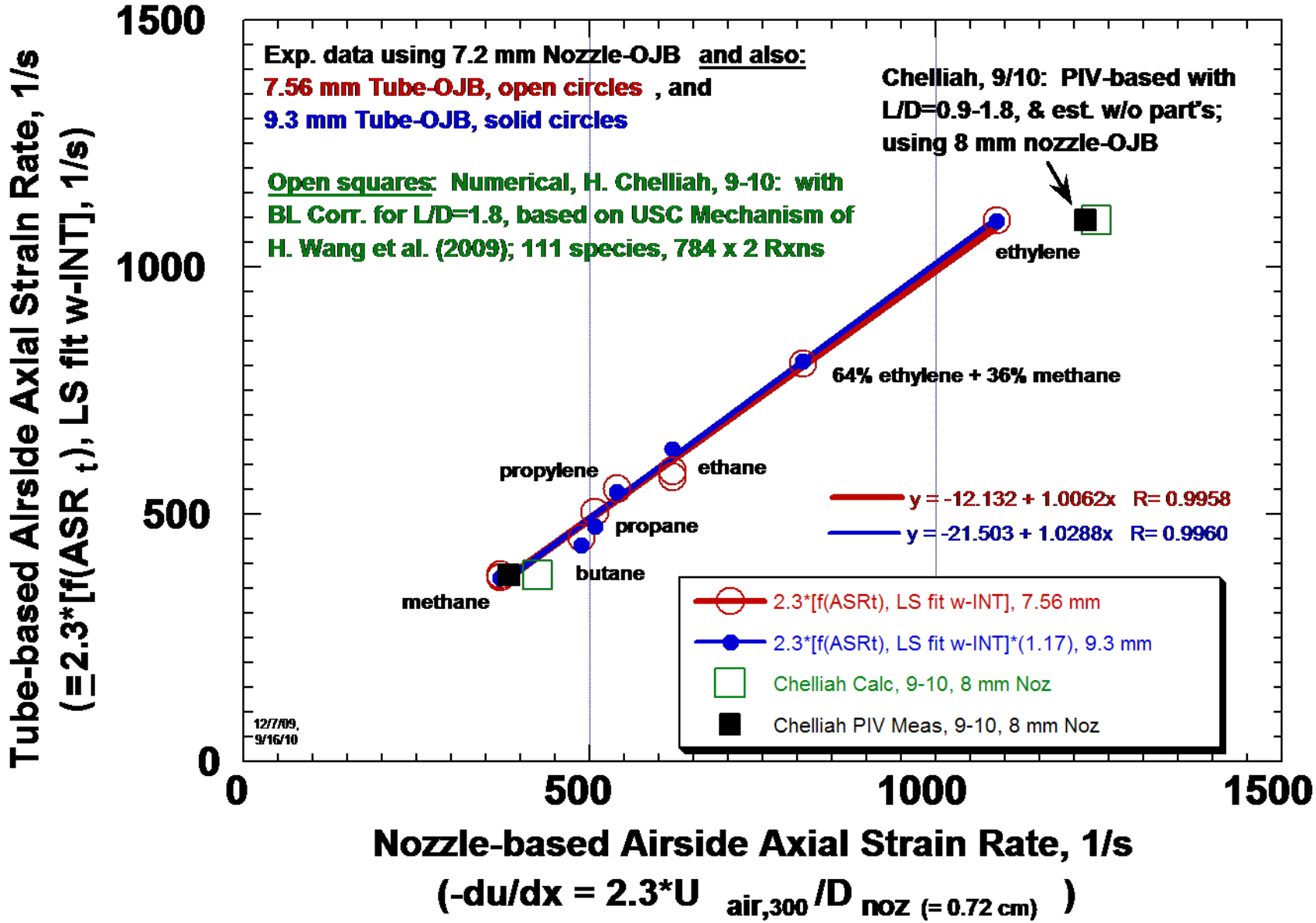
(1) Use of 2.3 factor (= 2 * 1.15) corrects nozzle-based ASR_n data, *and*

(2) Use of best empirical LS fit of ASR_n vs. ASR_t for extensive extinction data on 7 gaseous HCs,

$$ASR_n = -37.12 + 2.533 * ASR_t ,$$

allows the use of **$2.3*(-37.12 + 2.533 * ASR_t)$** to represent Tube-OJB ASR_t data on an equivalent $2.3 * ASR_n$ scale.

Comparison of Experimental and Numerical Strain-Induced Extinction Limits for Fuel vs. Air Counterflow Diffusion Flames at 1 atm, Using Best Estimates of (local) Airside Axial Strain Rate



Conclusions Re: Extinction Limits for C_2H_4 and Simple HCs

- The new ASR extinction limits for 7 gaseous HCs agree exceptionally well with the author's previous (2008) results derived from a slightly smaller Tube-OJB.

- (1) New independent global extinction, and refined PIV axial Strain Rate **measurements** at UVa for C_2H_4 and CH_4 OJB flames; *and* (2) Refined **numerical simulations** at UVa for C_2H_4 and CH_4 extinctions, using a revised 2009 chemical kinetics model (USC), agree quite closely with present experimental results on a deduced "absolute" axial SR scale (both are ~ 12 % higher for C_2H_4).

- The present agreement helps justify development of a reduced kinetics model (with ~ 30 species) that will permit detailed numerical simulations of flameholding in HIFiRE-like scramjet combustor designs.

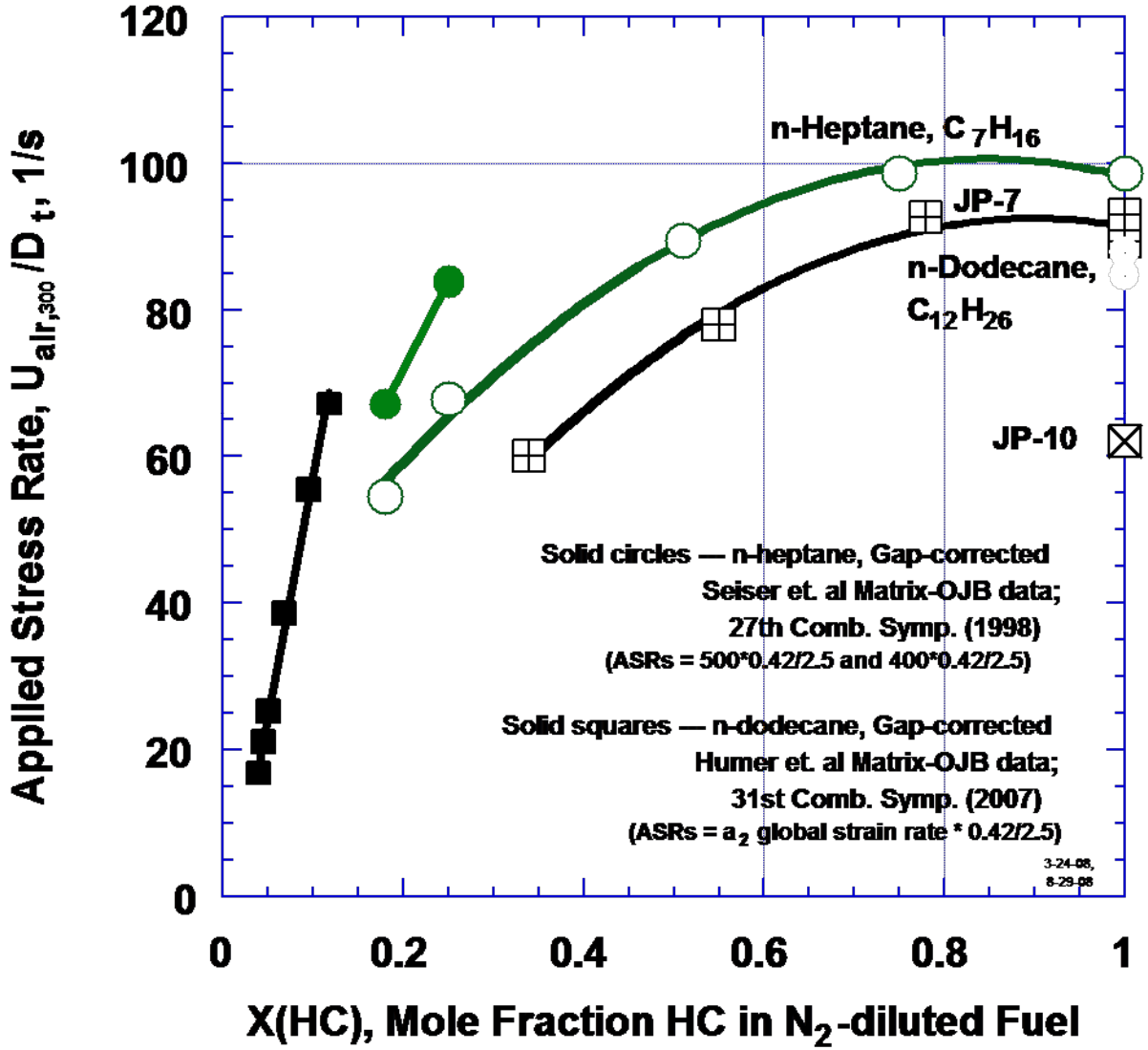
Extinction of Non-Premixed, Undiluted Vaporized-HCs vs Air;

and

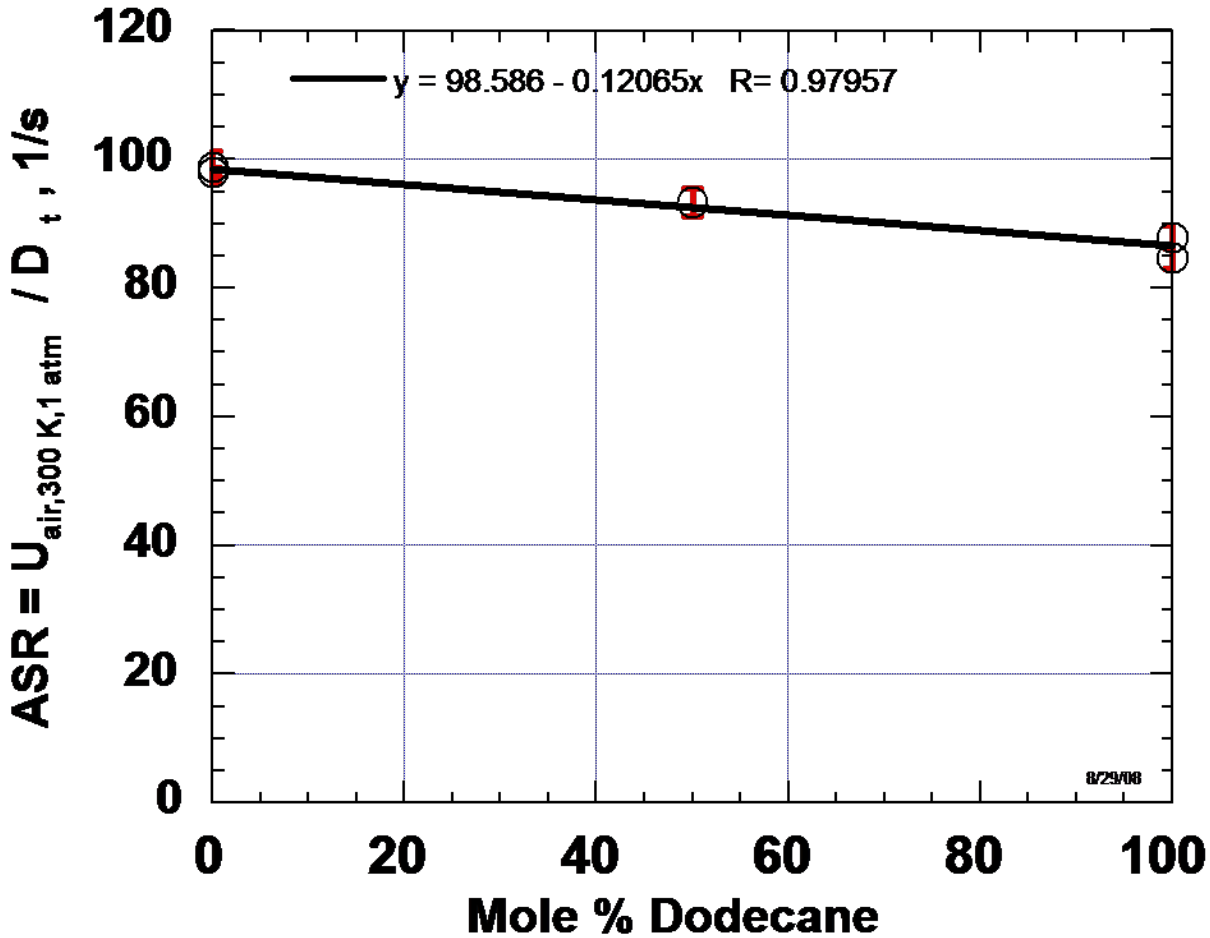
Consolidation of Results from 7 Simple Gaseous HCs

with Results from 11 Vaporized HCs, up to Tetradecane.

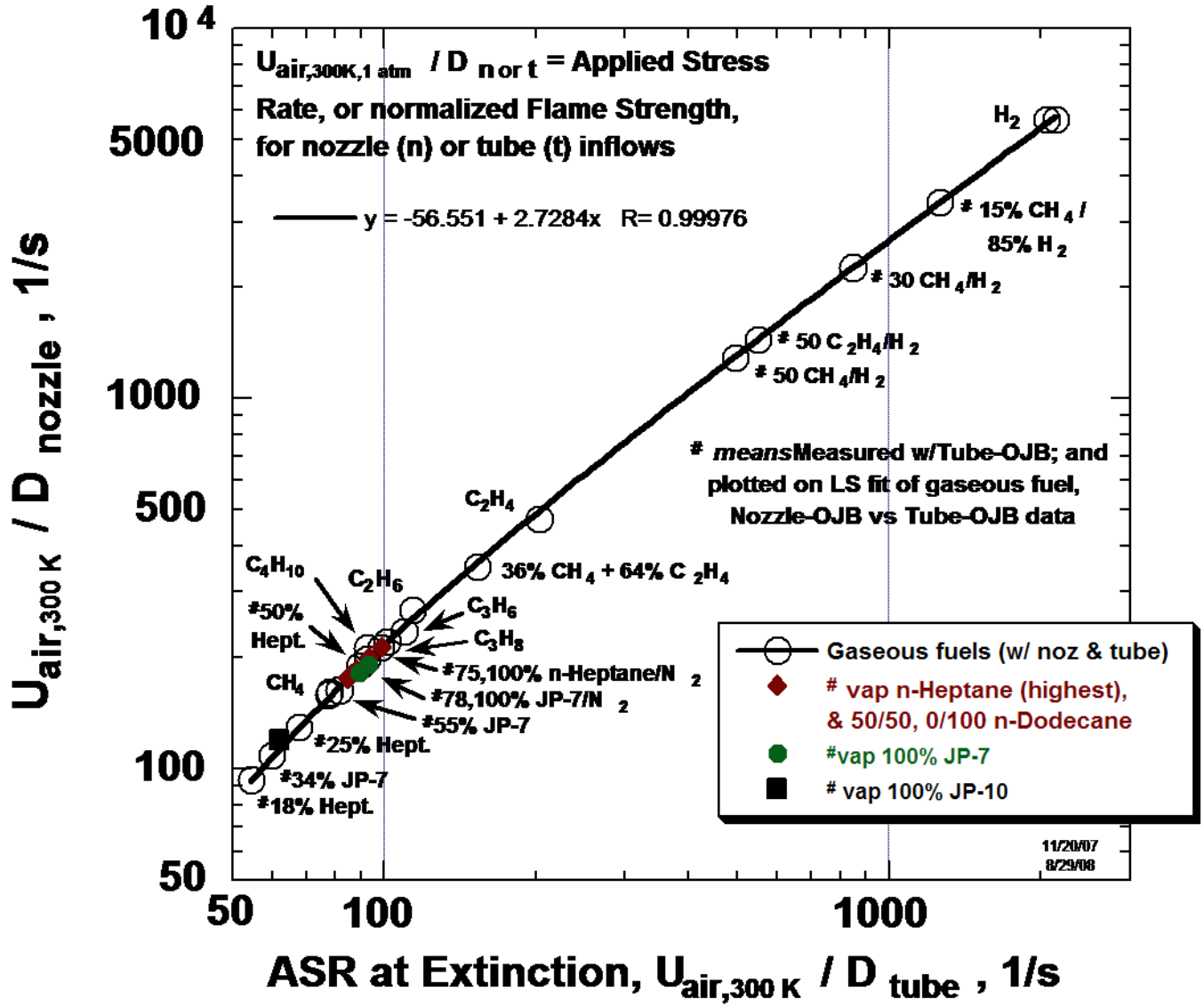
Extinction of N_2-diluted n-Heptane and n-Dodecane, and JP-7 vs Air CFDF's, using 7.5 mm Tube-OJB with Batch Vaporizer, and Comparison with Gap-Corrected UCSD Matrix Burner Data



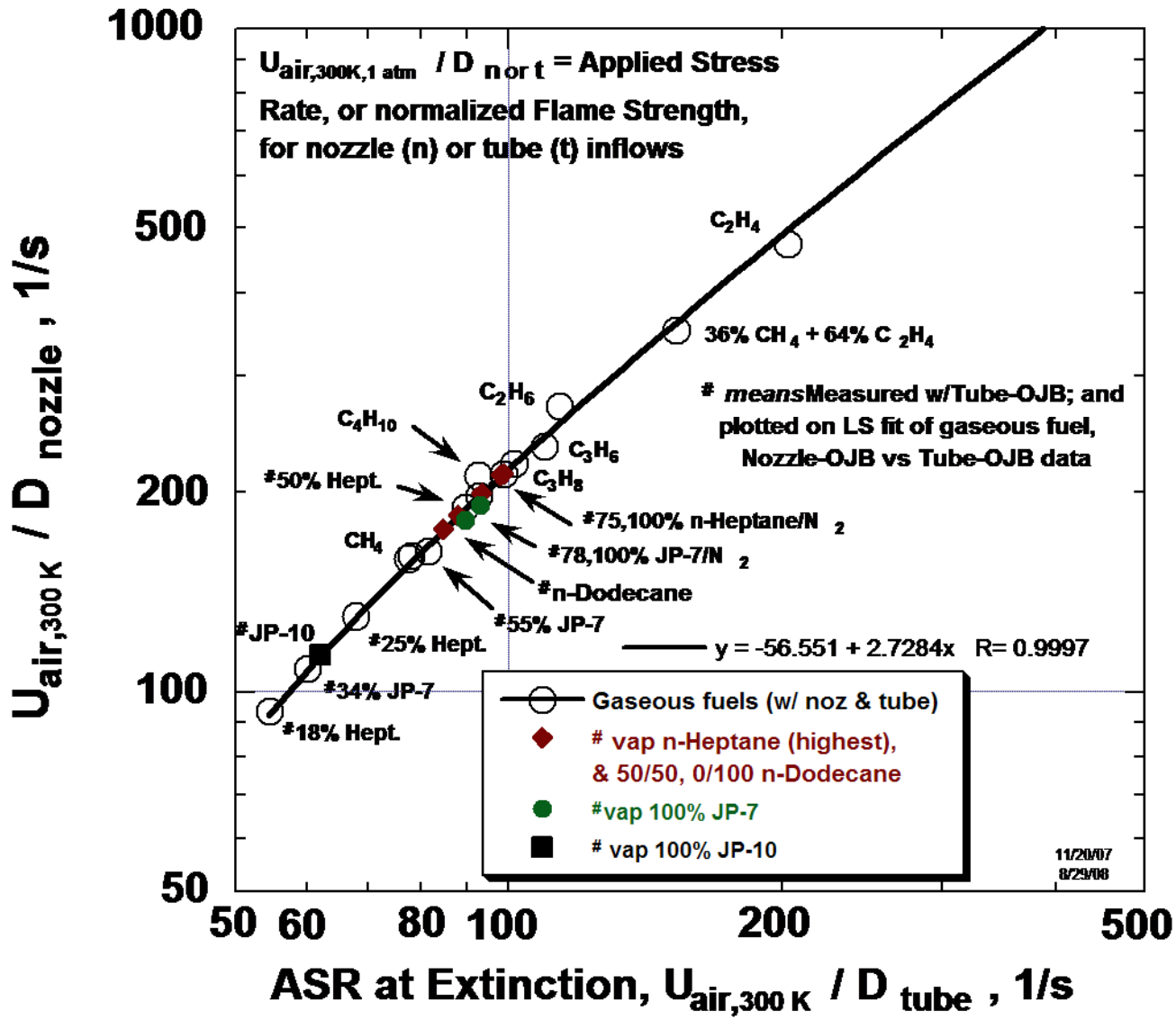
ASR at Extinction for Vaporized n-Heptane + n-Dodecane Mixtures vs Air Counterflow DFs, using "Minimally Heated" Vaporizer System to feed 7.56 mm Tube-OJB, 1 atm



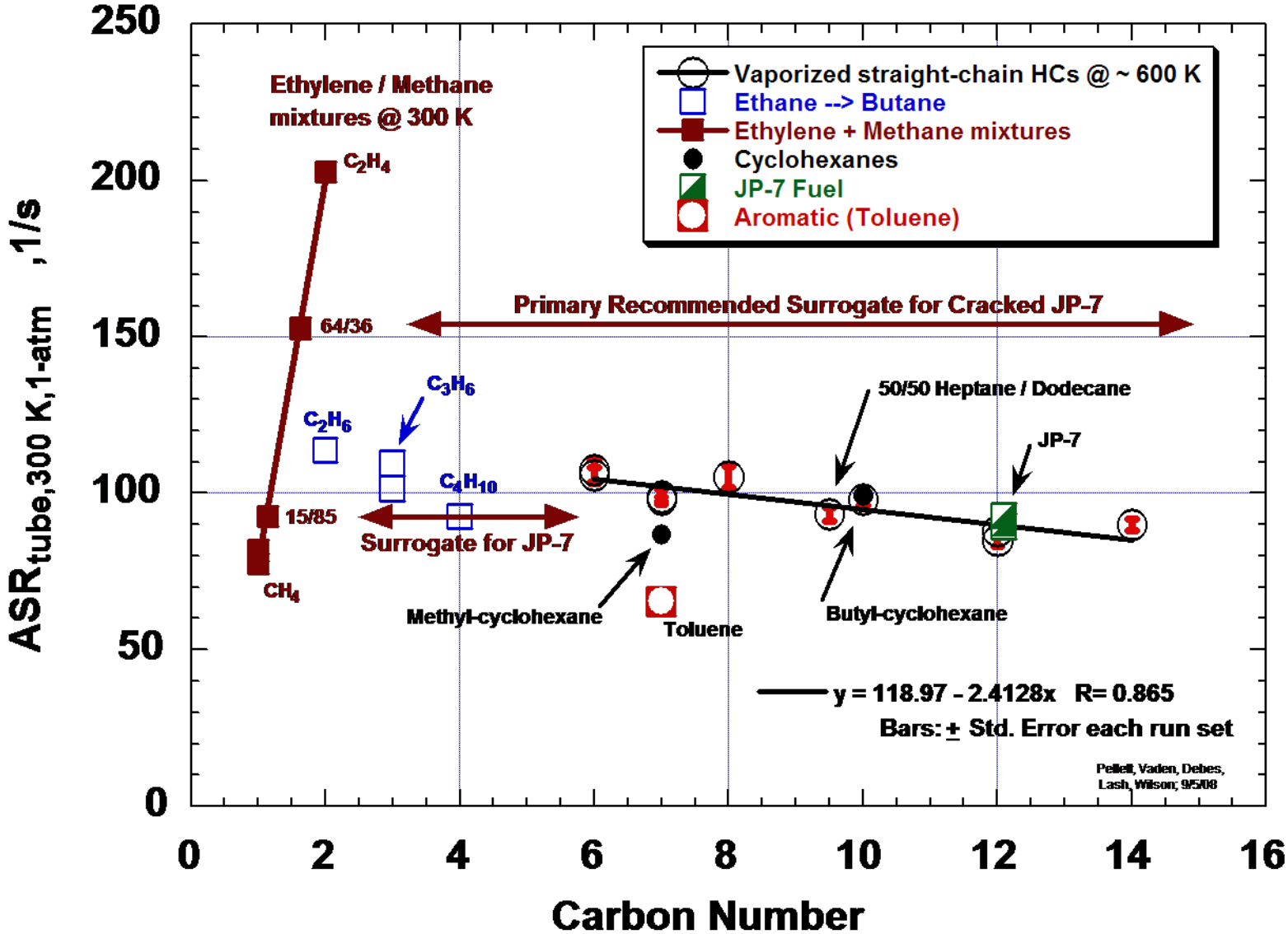
OJB-Extinction-Limit "Idealized Flameholding Scale" from Convergent-Nozzle- and Tube-OJBs, for: JP-10, n-Dodecane, JP-7, n-Heptane; and Methane, Butane, Propane, Propylene, Ethane, 36% CH_4/64% C_2H_4, Ethylene, and H_2 vs Air CFDFs



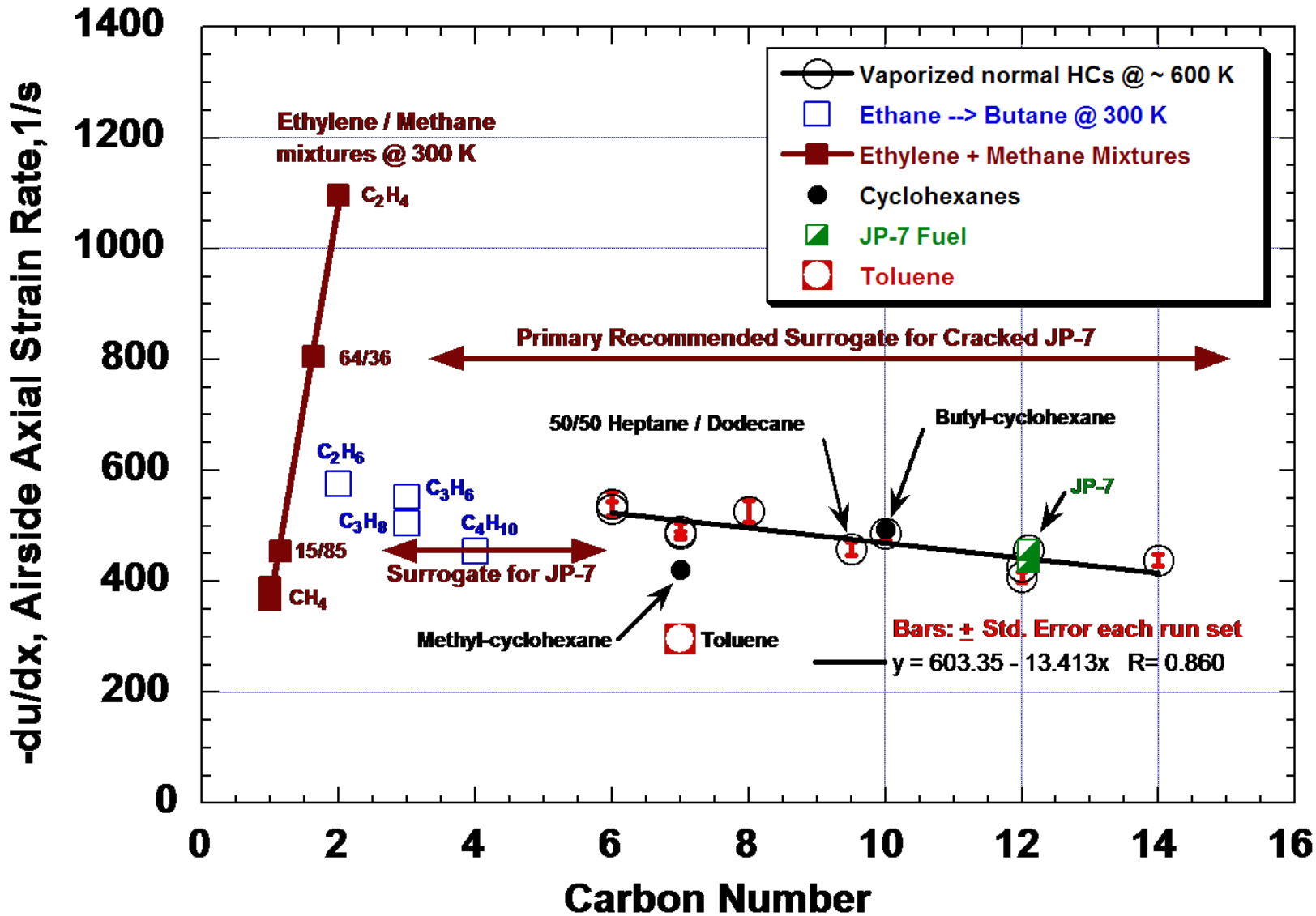
OJB-Extinction-Limit "Idealized Flameholding Scale" from Convergent-Nozzle- and Tube-OJBs, for: JP-10, n-Dodecane, JP-7, n-Heptane; and Methane, Butane, Propane, Propylene, Ethane, 36% CH_4/64% C_2H_4, Ethylene, and H_2 vs Air CFDFs



Applied Stress Rate (Extinction) for Gaseous & Vaporized-Liquid Hydrocarbons vs Air, using "Minimally-Heated" 10.6 L System to Feed 7.56 mm tube-OJB @ 1 atm



Best Estimate of Airside Axial Strain Rate for Extinction of Gaseous & Vaporized-Liquid Hydrocarbons vs. Air, using "Minimally-Heated" 10.6 L System to Feed 7.56 mm Tube-OJB @ 1 atm



Conclusions Re: Extinction of Gaseous and Vaporized HCs

Consistent scaling of ASR_n and ASR_t results has been obtained.

The ASR_t results appear basically consistent with expected trends as a function of molecular structure.

The present ASR_t extinction results on gaseous and vaporized HCs are now transformed as best empirical estimates of the (cool) airside axial strain rate at extinction for the (non-premixed) HC vs. air flames.