Use of Kinetic Models to Predict Fuel Impact on Engine Performance

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4th Annual Fuel Research Meeting

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Air Force Research Laboratory

Background

- Secure supply
  - Military needs guaranteed fuel supply in time of war
- Global Warming:
  - Combustion of fossil-derived fuels
  - Combustion emissions (soots/particulates)
- Physics-based combustor models
  - Existing models barely sufficient for design predictions
- Physical vs. chemical effects
  - Physical effects presumed to dominate
- Complexity of fuels
  - Large number of species
  - Unknown/uncertain reaction rate laws
- DoD needs
  - AF – 50% utilization of alternative fuels by 2016 (in US)
  - Navy – Sailing the 'Great Green Fleet' by 2016
  - SERDP – Understand impact on emissions

Objectives and Outline

Objectives:

- Apply methods/tools that can incorporate both physical and chemical effects to predicting impact on engine performance

Outline:

- Recommendations from 2010!!!!
- Review general modeling approach
- Applications to
  - Lean blow-out (review)
  - Altitude Relight
  - Emissions
    - Unburned hydrocarbons
    - Soot

Challenge Problems

- Summary
- Recommendations

Recommendations/Needs – from 2010!!!!!

- Validated mechanisms that predict ignition and extinction
  - particularly aromatics and cycloalkanes
- Broader/validated tool for selecting surrogates that match properties of petroleum fuels and synthetic fuels
- Soot growth models incorporating effect of PAH surface addition
- Models that describe HC emissions fingerprint and changes with fuels
- Inclusion of ignition criteria for certification of alternative fuels
  - What should be the standard?
  - Incorporate physical effects?
- New ignition data at low pressure needed
  - Fuel components
  - Jet Fuel
  - Alternative jet fuels

Tools for Assessing Fuel Impact on Performance

Alternate Fuel: Phys & Chem Prop

Surrogate for alternate fuel

Detailed Kinetics for Surrogate

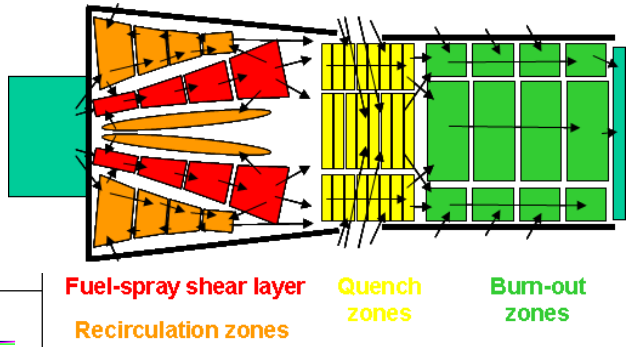
Selection of physics-based tools sets

Simulations

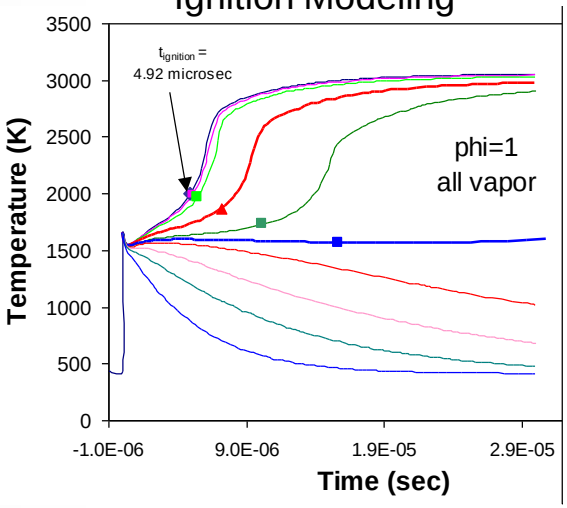
Probable impact on combustor

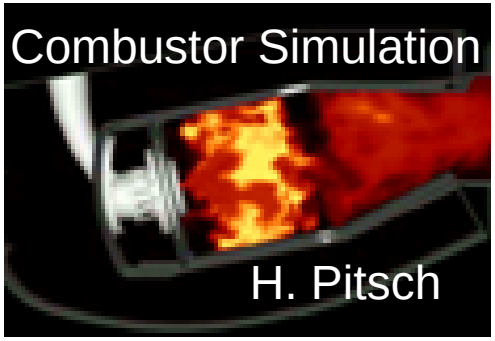
Interpretations and Engine Impact

Emissions



Ignition Modeling





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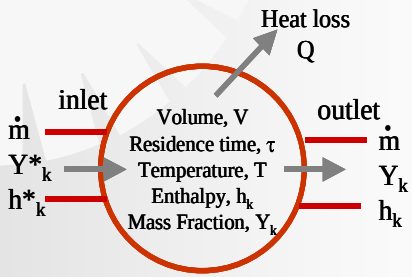
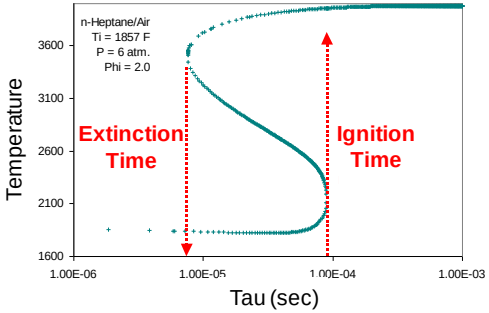
Modeling Methods – Physical Models

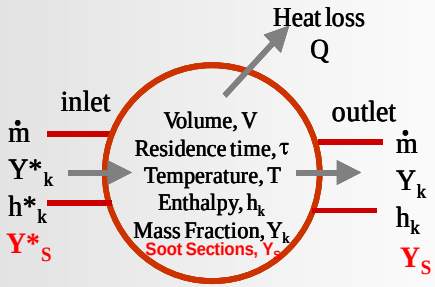
Simplified, kinetics-based model of physical problem (CHEMKIN based)

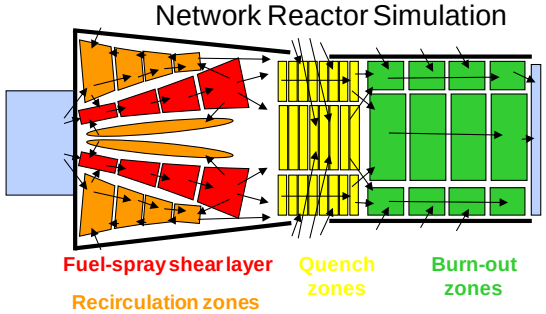
- Lean Blow Off – Extinction of a 'Perfectly Stirred Reactor'





- Altitude Relight – Revised SENKIN with added mixing and vaporization
  - Initial energy provided by prescribed spark
- Soot – (PSR) Network Reactor Code with coupled soot equations





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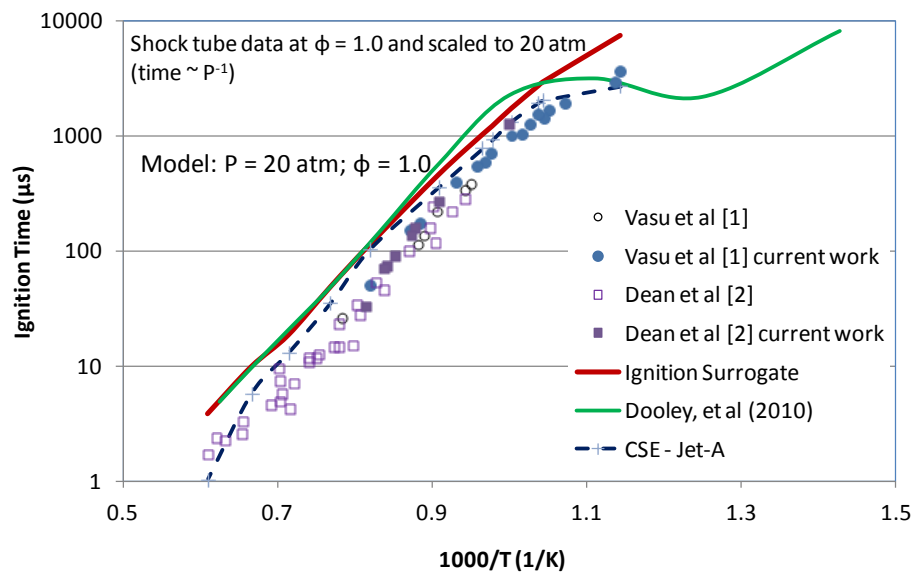
Surrogate Fuel Identification - Demonstration

Based on HC classes

	ONR Liq vol fraction	ONR Mass fraction	ONR Molar fraction	Mil Spec Min	Mil Spec Max	PQIS Database Min	PQIS Database Mean	PQIS Database Max
n-heptane	25	0.227	0.226					
iso-octane (2,2,4-trimethylpentane)	20	0.184	0.161					
methylcyclohexane	35	0.358	0.364					
toluene	20	0.231	0.249					
grams/cc		0.752		0.775	0.84	0.796	0.817	0.837
MW		99.712						
H/C		1.899		1.85		1.85	1.9	2.1
SP(mm)		21.14		19.00		19	21	26
HtComb (MJ/kg)			43.31	42.60		42.90	43.11	43.40

Surrogate – blend of reference Fuels obtained by matching H/C, Smoke point, Ht. of combustion

1) Kinetics model (ignition surrogate) selected from Westbrook, et al
2) Compared to surrogates and kinetics proposed by others
3) Benchmarked model against Vasu et al (C&F) expts
4) Kinetics models/surrogates predict ignition times a factor of two too long



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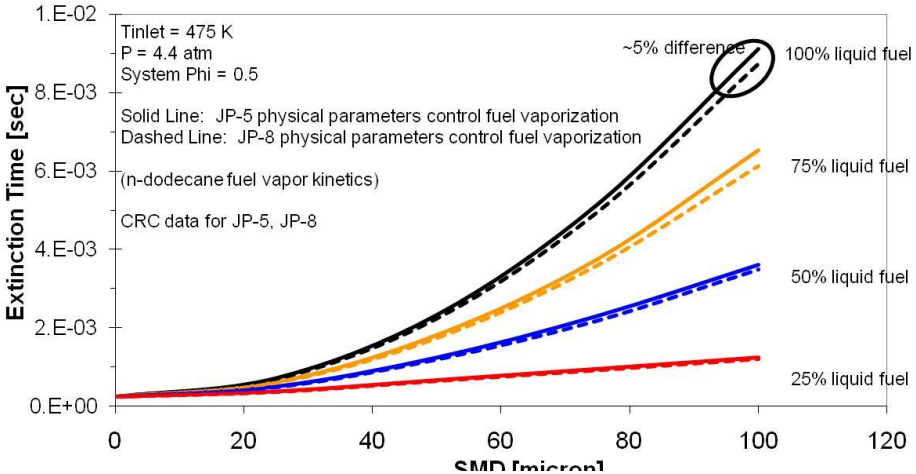
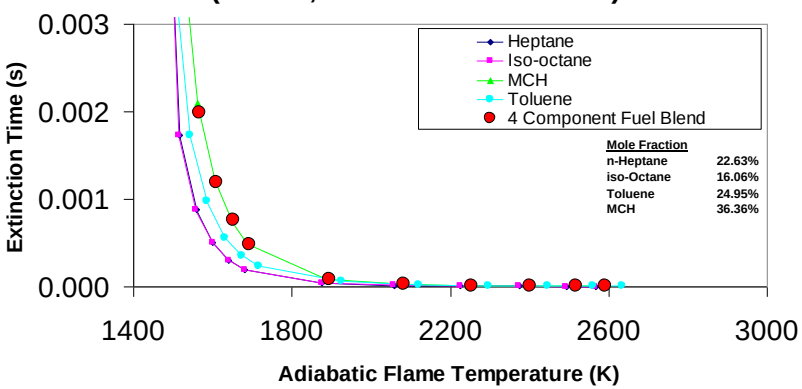
Observations from LBO Simulations

Based on PSR Extinction Times

- Small differences due to physical effects JP-8 to JP-5
- One fuel component had longer PSR extinction times – and controlled surrogate extinction time. (Perhaps due to uncoupled reaction mechanism)
- Most mechanisms are not (or poorly) validated against flame extinction
- Better reaction models for cycloalkanes are needed



Comparison of Extinction Behavior for Various Fuels & Representative Fuel Blend (10 atm, 750K Inlet Conditions)



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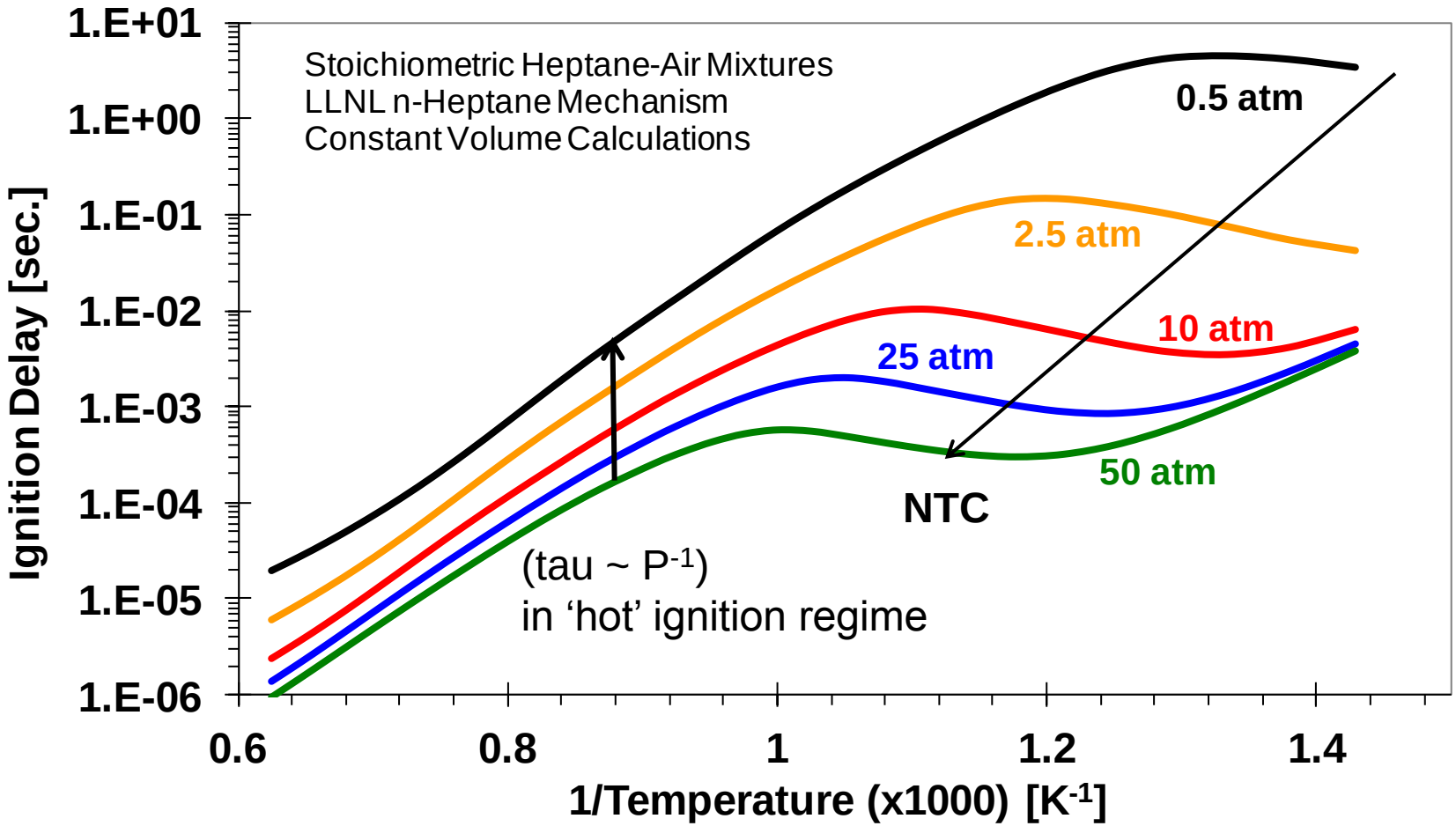
AutoIgnition: Strong pressure dependence

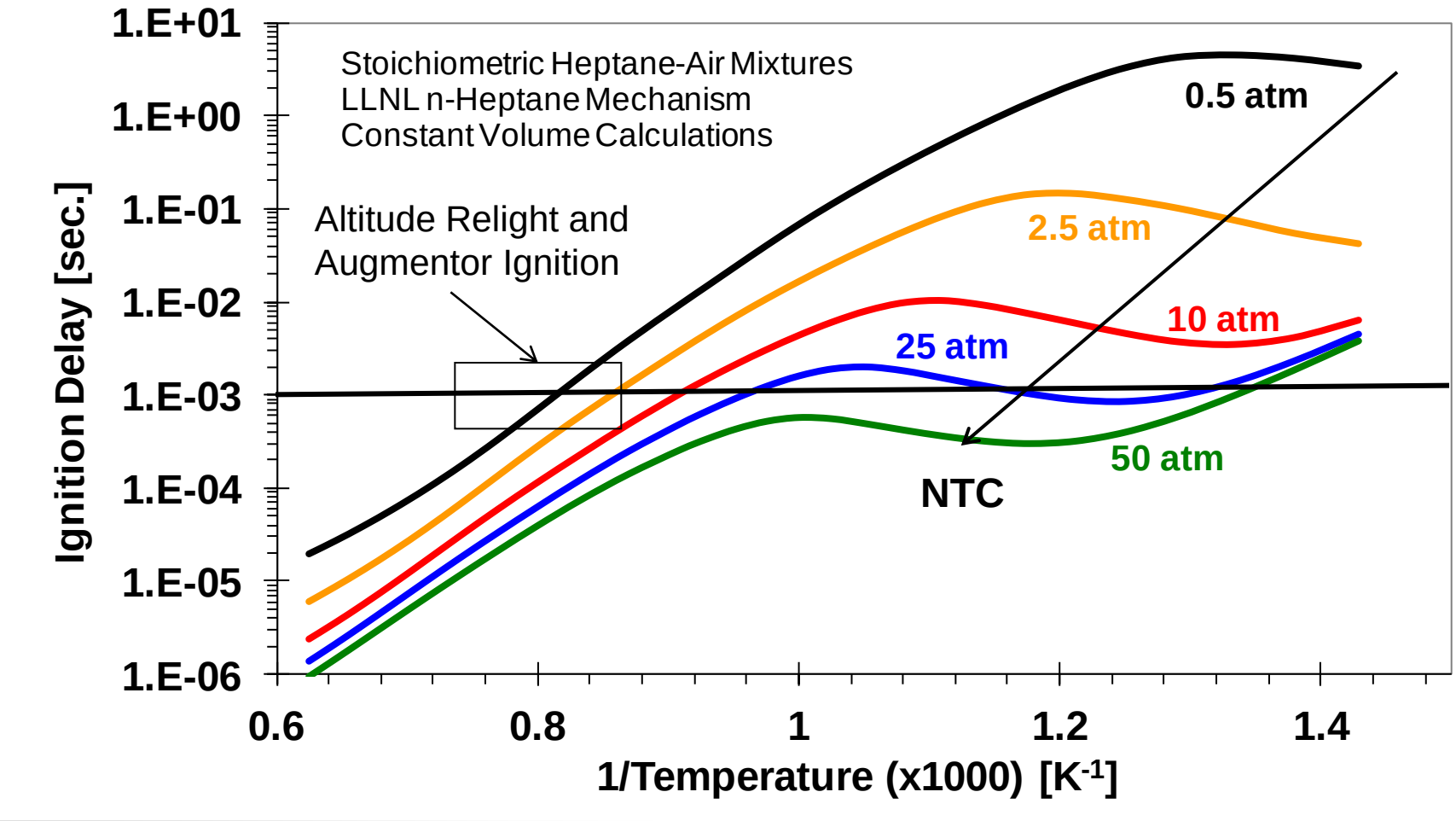
Review from last year

NTC shifts to higher temperatures with increased P



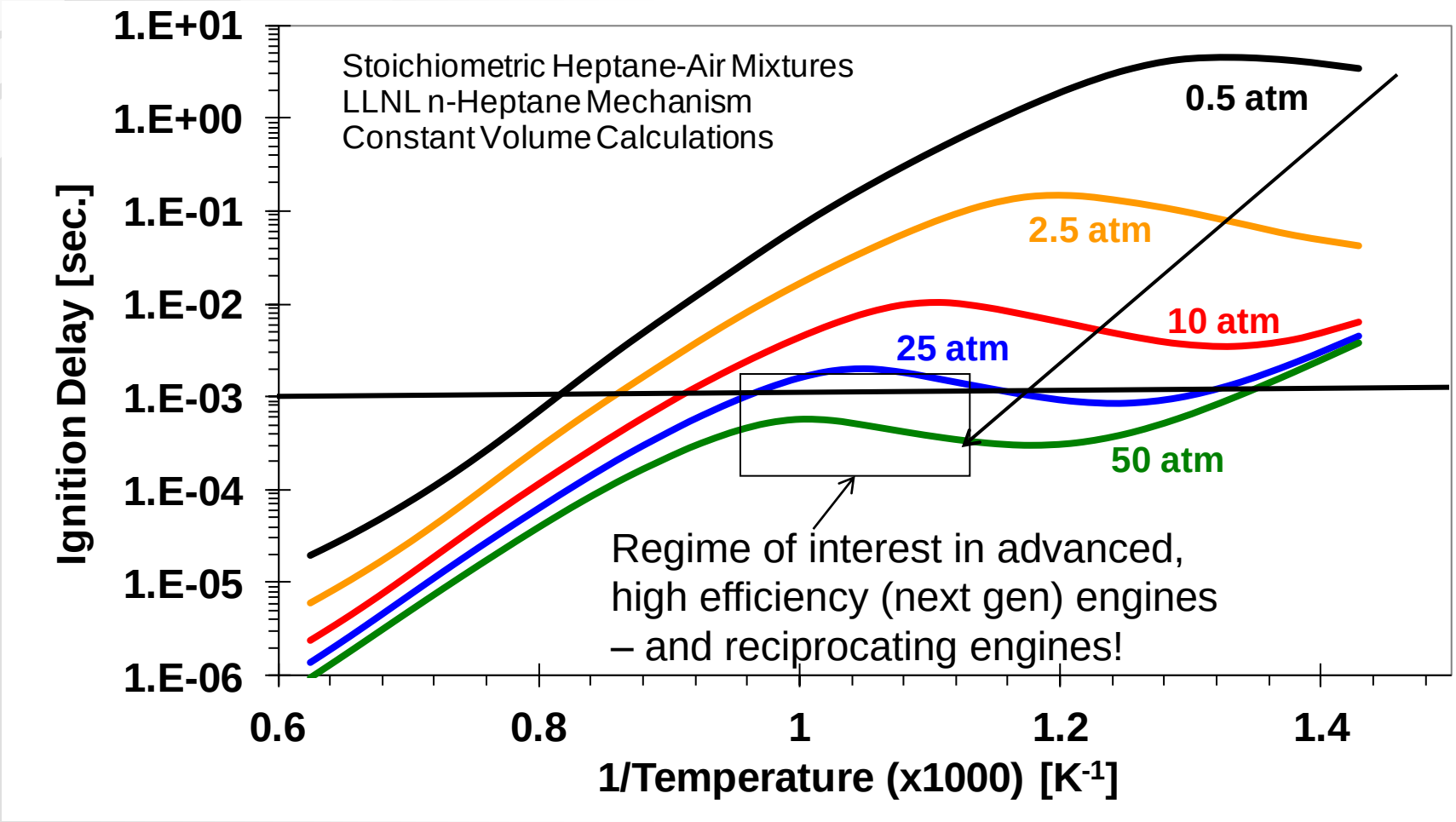
AutoIgnition: Strong pressure dependence

NTC relatively region unimportant for present day engines



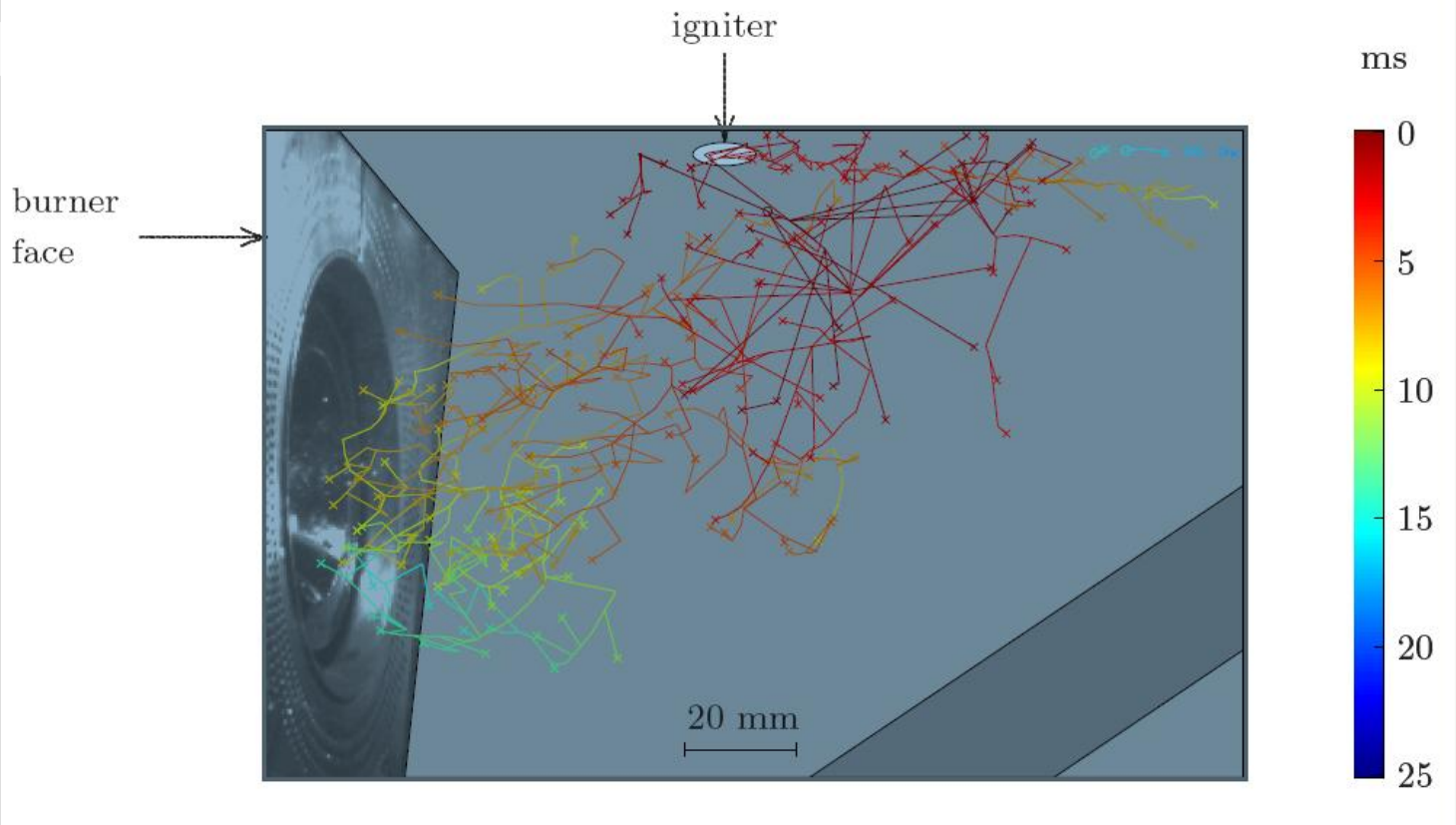
AutoIgnition: Strong pressure dependence

NTC of increased interest with increased P



Challenge Problem: Altitude Relight

Spark survival of >10 msec followed by ignition is inconsistent with mixing/cooling rates



Spark energy should dissipate in 1-3 milliseconds !

Explanation may be fuel-type dependent

Spark Trajectories from Reid, Rogerson and Hochgreb, AIAA 2008-957

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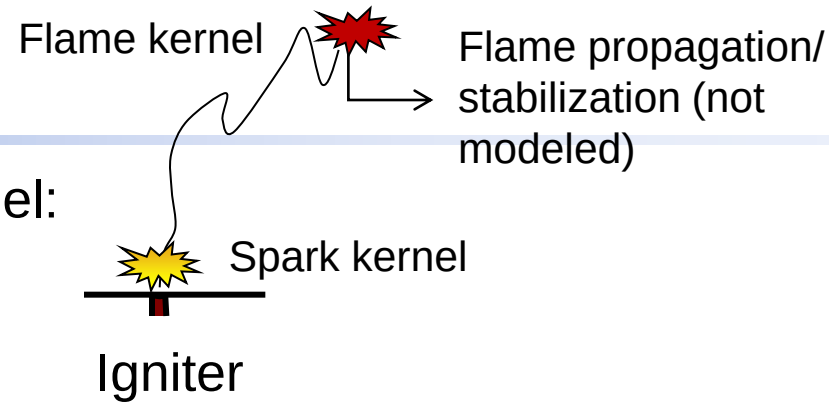
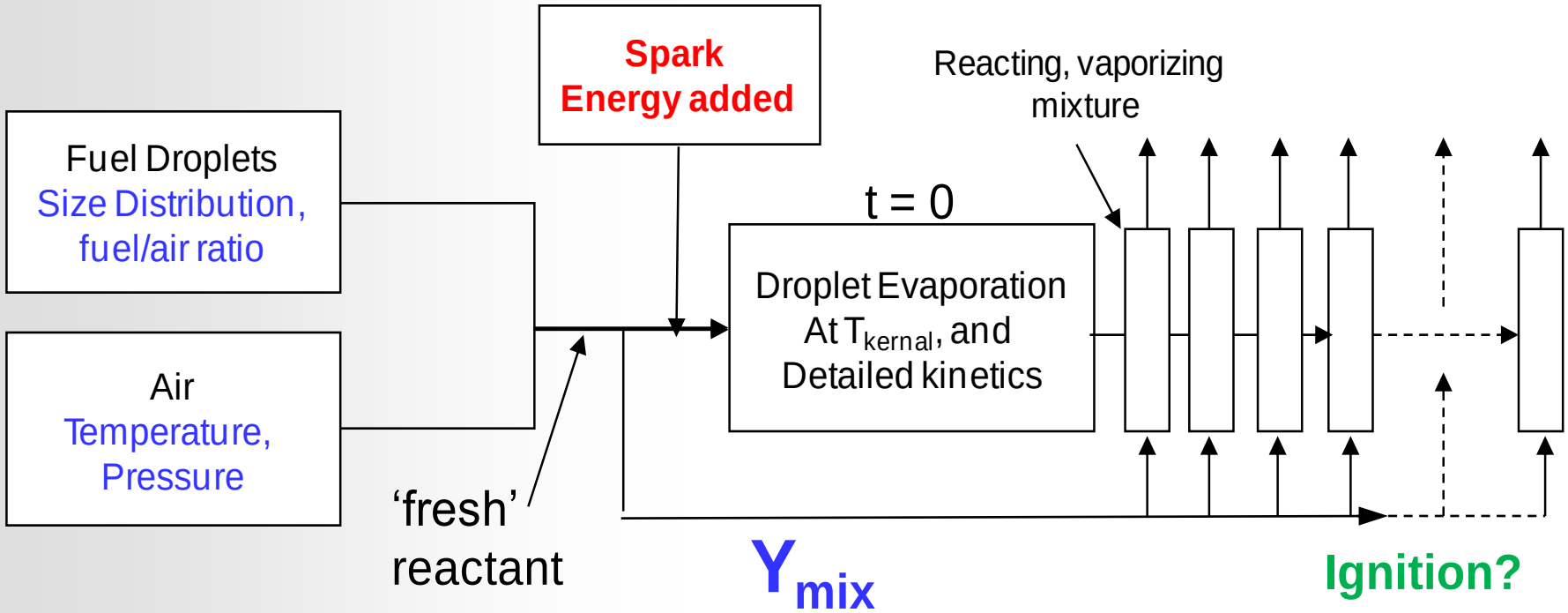
Flame Kernel Model



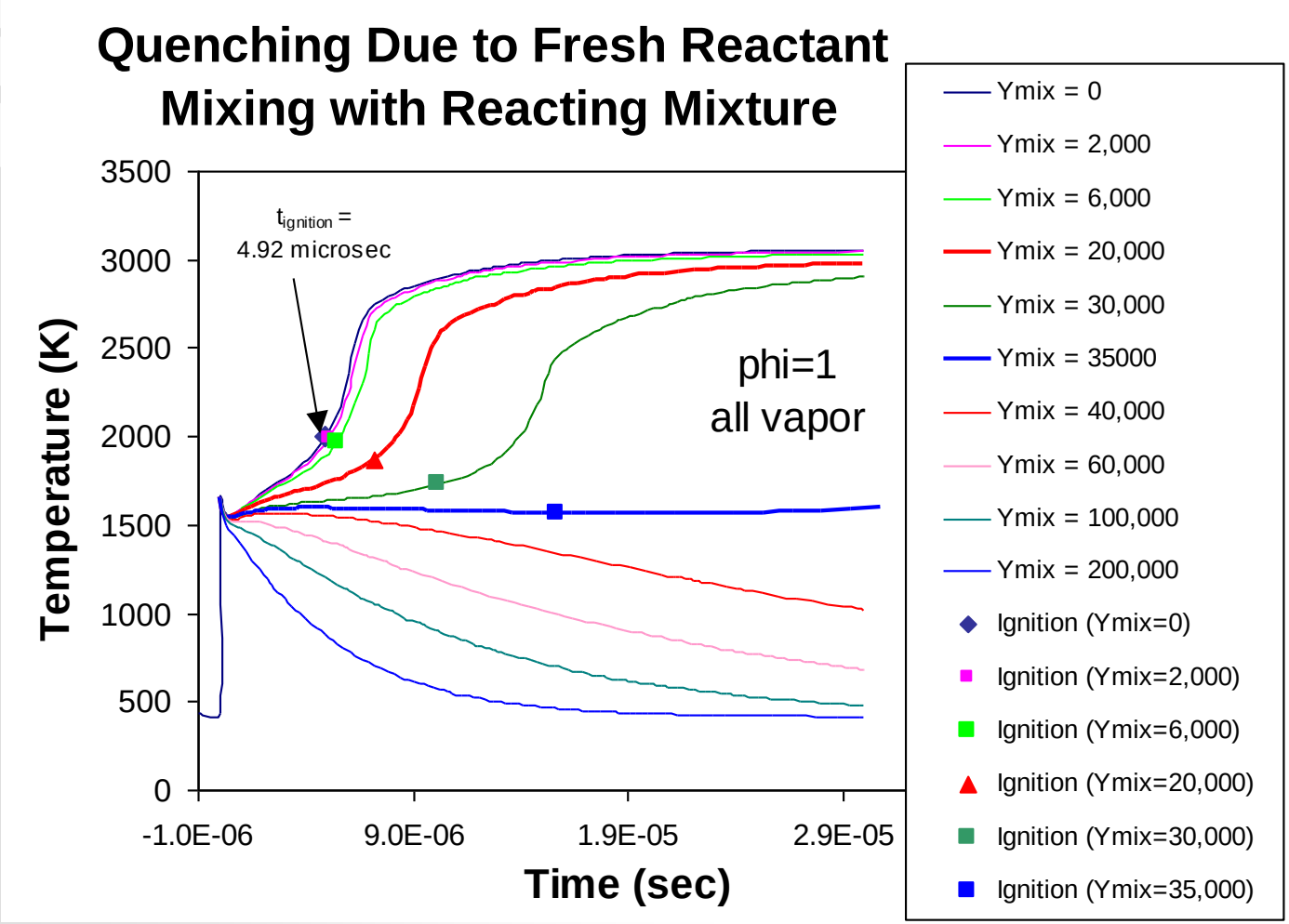
Coupled Kinetics/Mixing/Vaporization Model:

- Full detailed kinetics (SERDP surrogate)
- Specify SMD (drop size distribution)
- Specify mixing rate Y_{mix} (1/sec)
- Added energy – after early, rapid relaxation



Altitude Relight/Ignition Modeling – Mixing Effect

Turbulent Mixing can quench chemical reactions and inhibit ignition



Gaseous fuel: no vaporization

Example conditions:

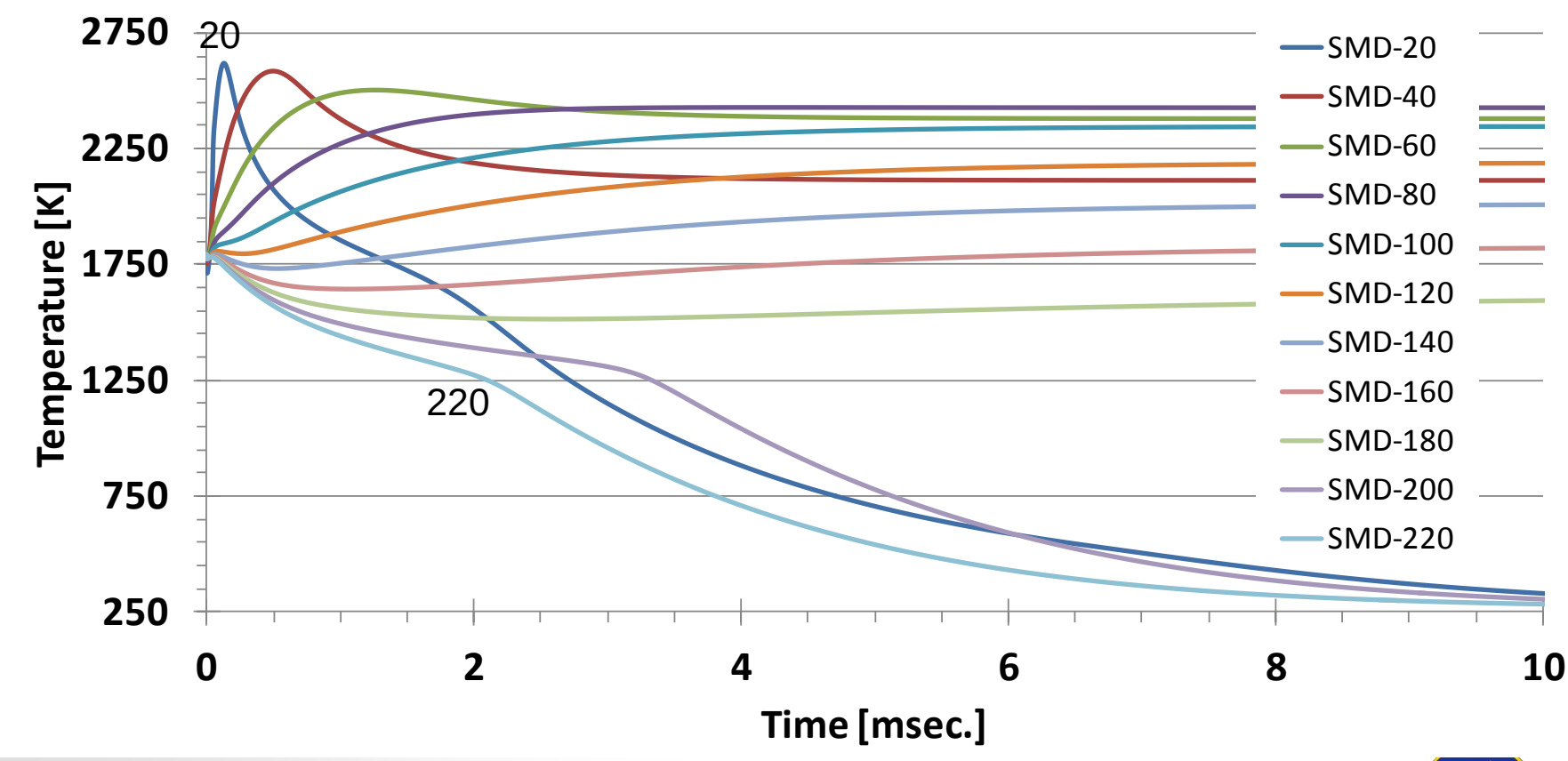
- Phi = 1
- FracL=0 (fuel vaporized)
- P=1.422 atm
- T=440.9 K
- E/M=943 J/gm

Altitude Relight/Ignition Modeling – Mixing/Vaporization

Coupled Mixing with Vaporization complicates inhibition (thermal quench)

All fuel initially liquid (variable Sauter Mean Diameter); Total phi = 3.5

T_{init} = 265K; P = 0.36 atm; Y_{mix} = 625 sec^{-1}



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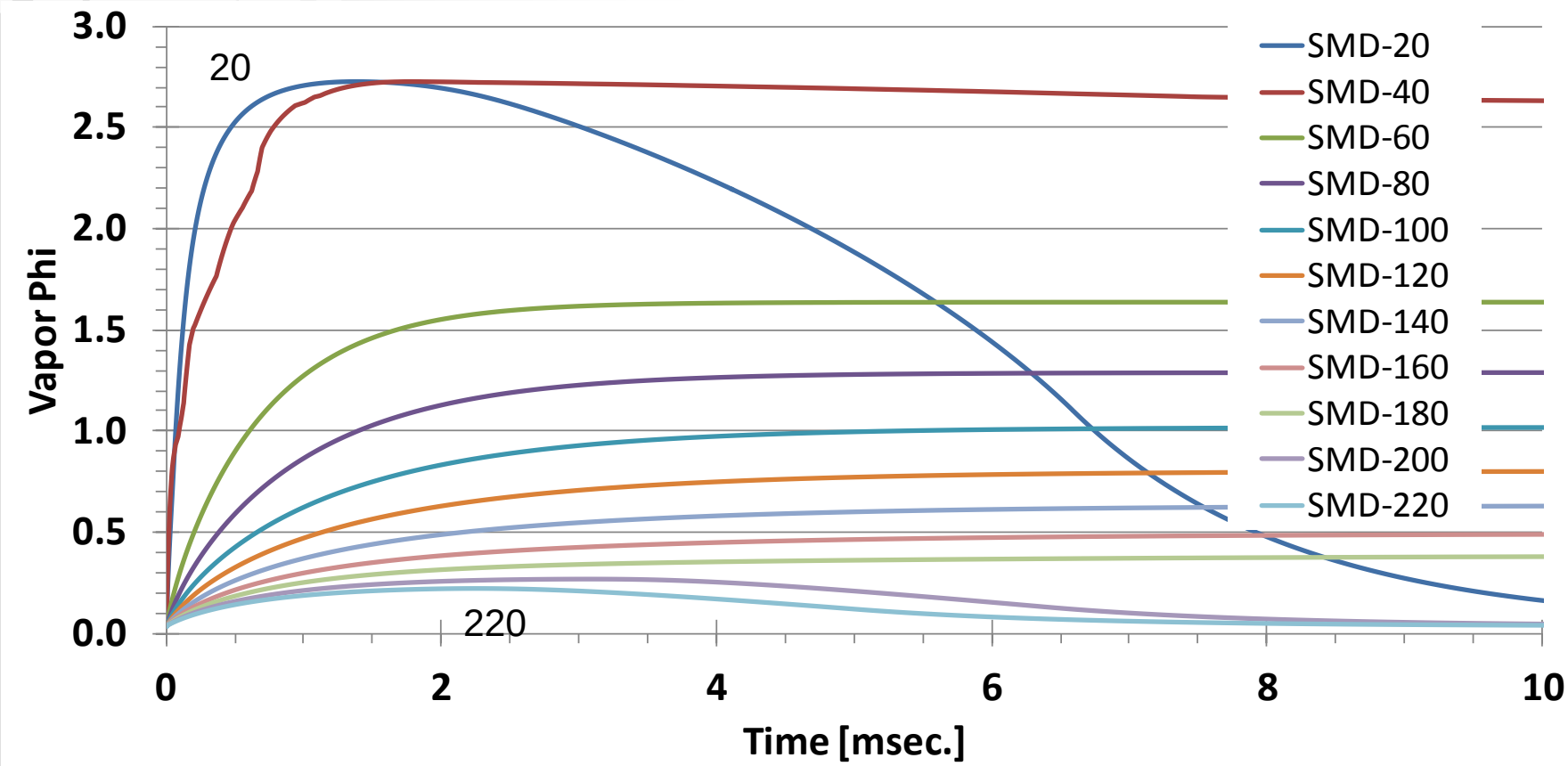


Prediction of Fuel Effects of Altitude Relight

Use fuel with range in ignition characteristics – accentuate effects

Identify conditions suitable for sustained kernel

SERDP Mechanism*

Three fuels

- 77% Dodecane/23% m-Xylene
- Dodecane
- m-Xylene

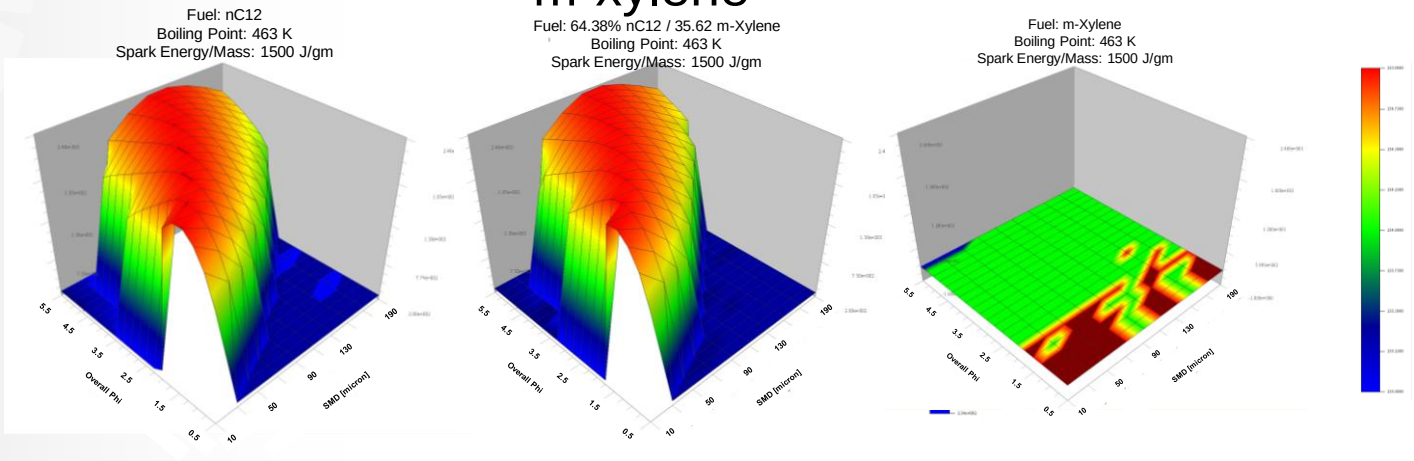
* UIC + USC + UTRC

SMD	fracL	phi	E/M
10	0.9	0.5	1300
30	0.93	0.75	1400
50	0.96	1	1400
70	0.99	1.25	1750
90		1.5	
110		1.75	
130		2	
150		2.25	
170		2.5	
190		2.75	
		3	
		3.25	
		3.5	
		3.75	
		4	
		4.25	
		4.5	
		4.75	
		5	
		5.25	
		5.5	

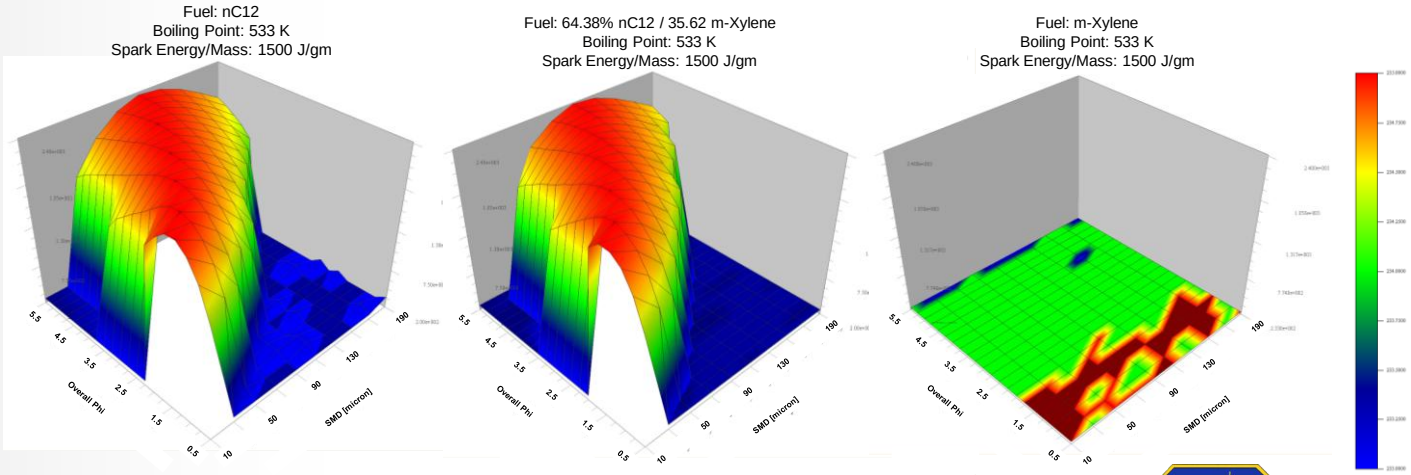
Final Kernel Temperatures for 1500J/gm

n-dodecane | n-dodecane/ m-xylene | m-xylene

$T_{boiling}$ = 463K (lower limit for Jet-A)



$T_{boiling}$ = 533K (upper limit for Jet-A, e.g., JP-5)



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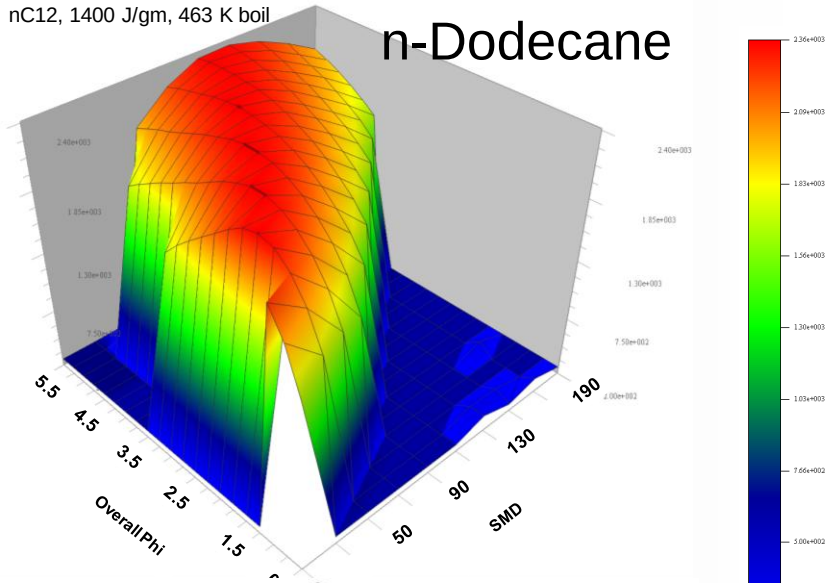
Sustained Kernels at 1400J/gm

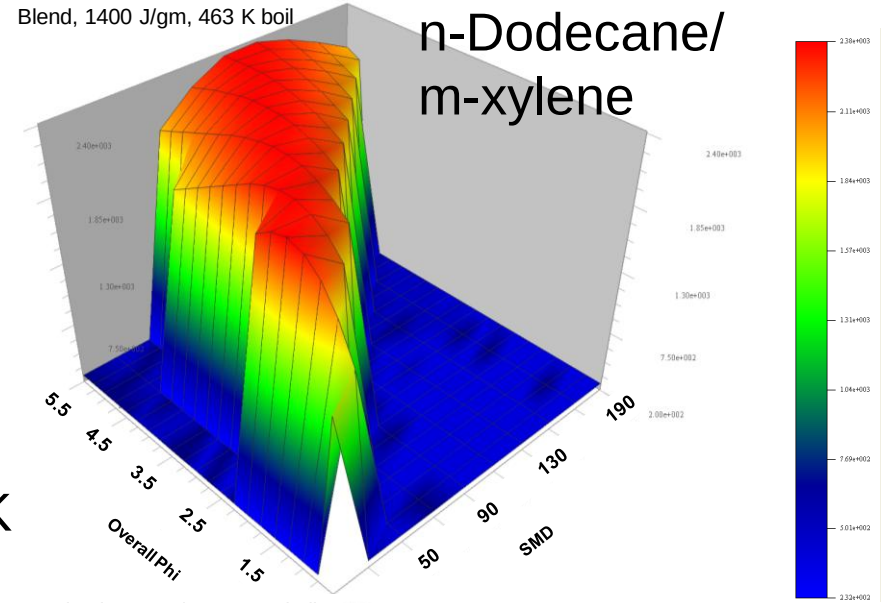
nC12, 1400 J/gm, 463 K boil

n-Dodecane



Blend, 1400 J/gm, 463 K boil

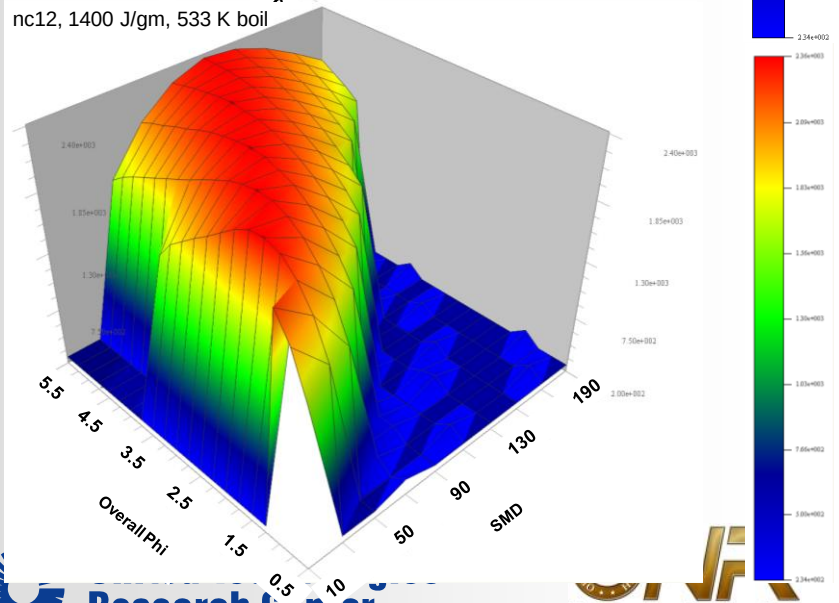
n-Dodecane/
m-xylene



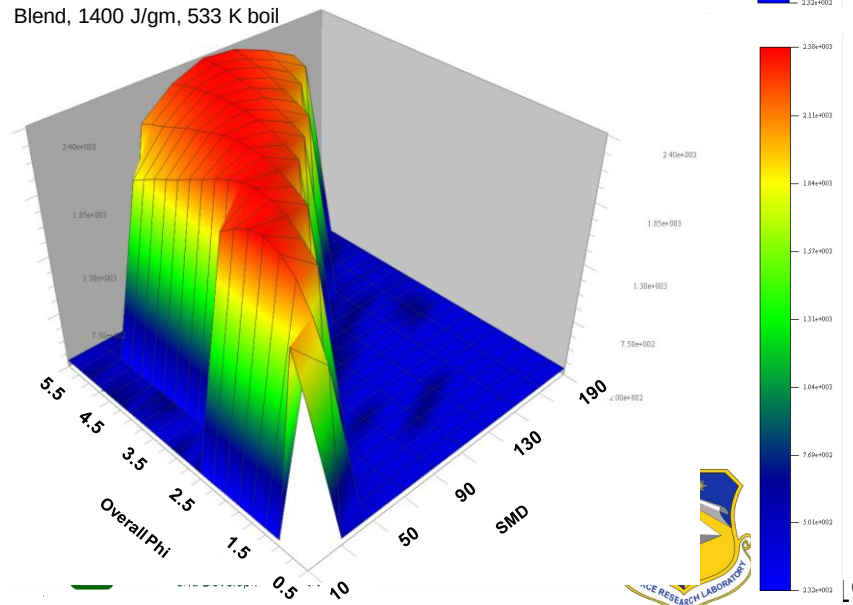
463K

533K

nc12, 1400 J/gm, 533 K boil



Blend, 1400 J/gm, 533 K boil



‘Statistical’ Analysis (arbitrary and unvalidated)

Statistics suggest dodecane will light more easily than the JP-8 surrogate (blend) and that lower boiling point fuels will light slightly easier

	Fuel					
	n-Dodecane		Blend Fuel		m-Xylene	
E/M (J/gm)	(463 K)	(533 K)	(463 K)	(533 K)	(463 K)	(533 K)
1300	0.0%	-	0.0%	-	-	-
1400	55.4%	54.1%	39.6%	38.6%	-	-
1500	62.9%	61.3%	61.2%	59.6%	0.0%	0.0%
1750	63.8%	62.3%	63.1%	61.5%	59.9%	58.0%
(trial size: 840 cases)						

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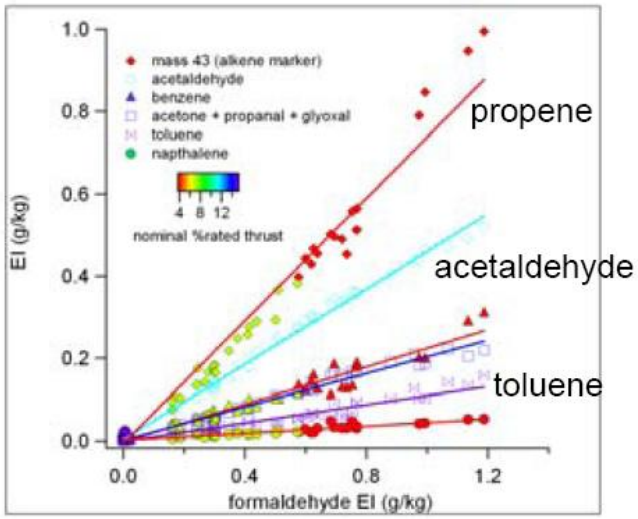
Challenge Problem: HC Emissions from Gas turbine Engines

Empirical evidence that emissions scale linearly – independent of engine or power

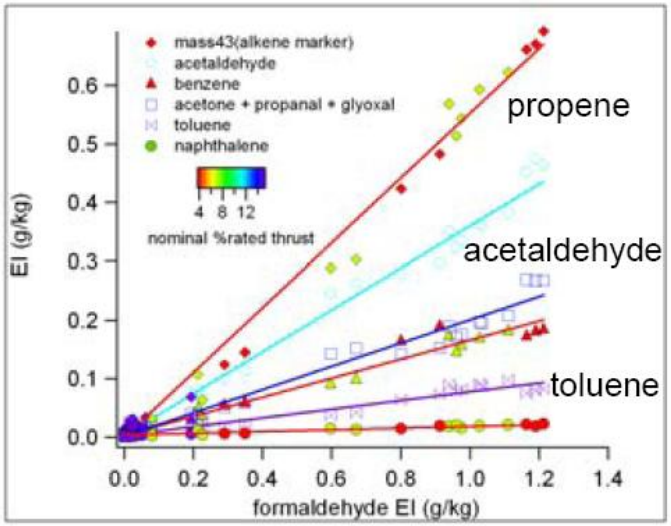
HC behavior is predictable and scalable

APEX 2



Includes 4 B737s.

APEX 3



Includes 1-B737, 2-B757, 1-A300.

Results from APEX 2 and 3

- What physical/chemical processes control this scaling?
- Can impact of alternative fuels on atmospheric pollution be anticipated?

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Approach

Identify chemistry and physics controlling scalability of HC emissions

Methodology:

- Utilize reactor-network formulation to simulate flowfield of burner
- Fuel used: 77% dodecane, 23% m-xylene (vol %) – SERDP mechanism
- Initially assumed "bulk flow" conditions (e.g., total flow rates, total burner volume, etc.)
- Modified to focus on conditions with measurable emission levels and those exhibiting scaling
- Approximate "Idle"/low-power conditions:

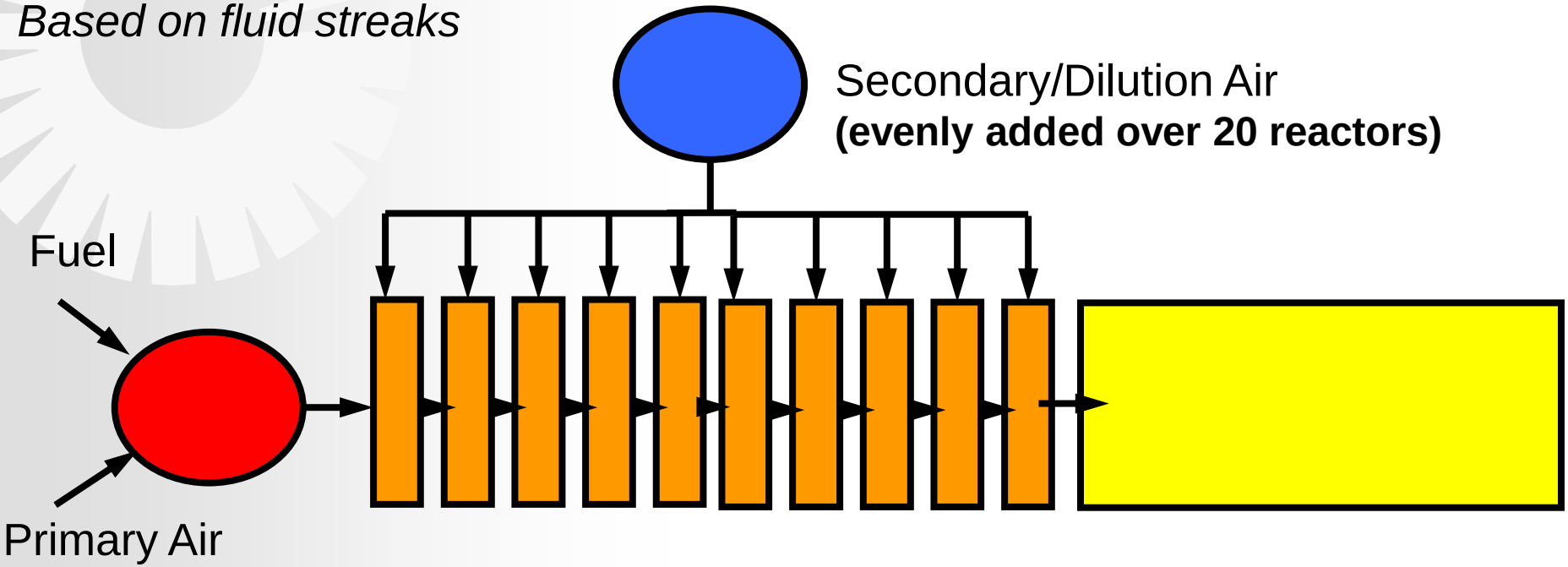
  P3 = 4.08 atm,

  T3 = 478 K

  Φ overall ~ 0.25

Network Construction for Refocused Analysis

Based on fluid streaks



Front-End

Residence time: .2-1.4 msec

Phi: 1.6-2.2

Quench Region

Residence time: ~0.05-0.005 msec

Exit Phi: 0.1-0.35

Burn-out

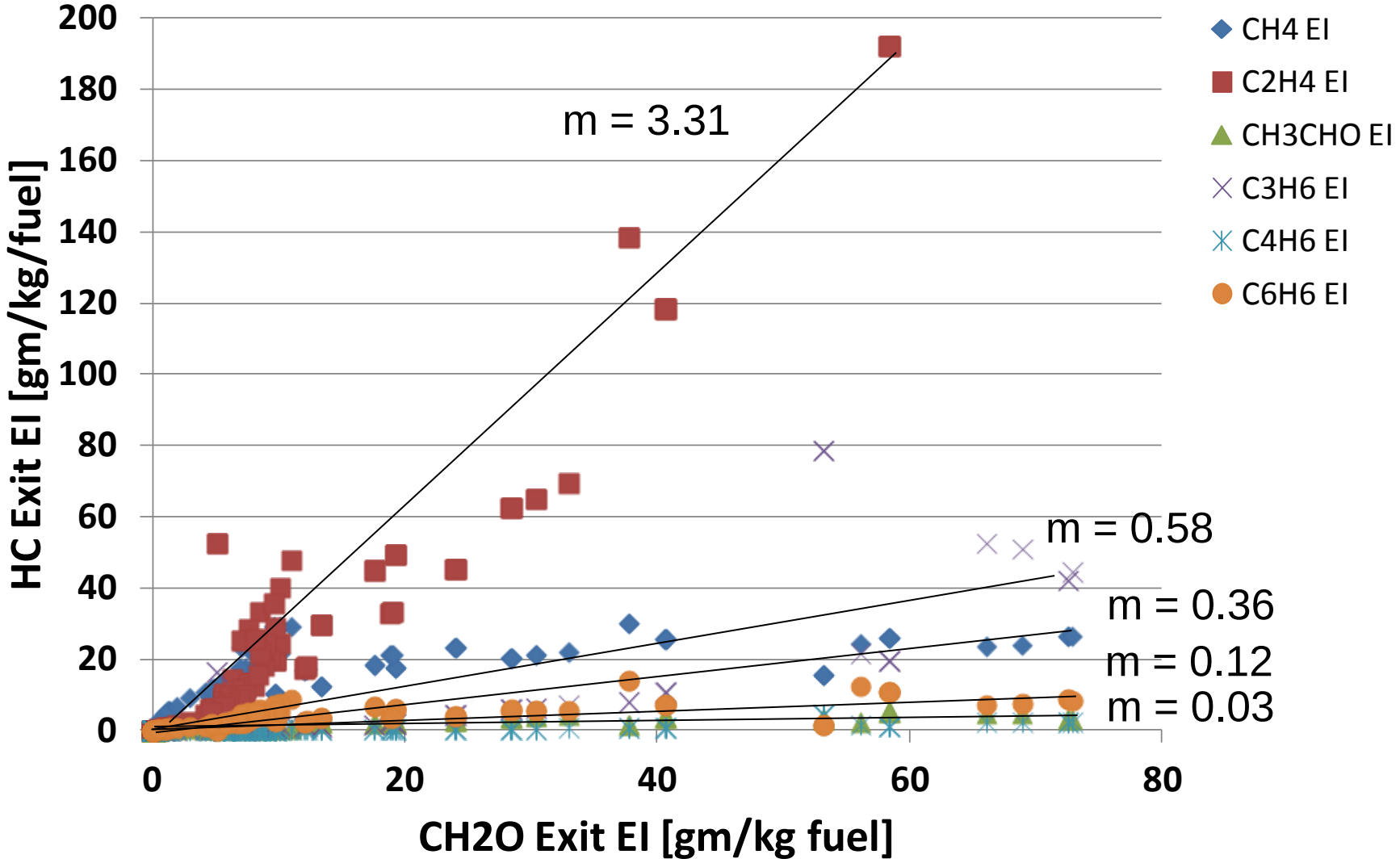
Residence time: *na*

Exit Phi: 0.1-0.35

Relaxed constraints relative to burner dimensions
(Emission levels expected to be high)

Results of Streak Analysis

'Correlations' enable estimating HC sensitivity to CH2O EI values



Results of Streak Analysis (for two surrogates)

Reasonable agreement for methane, ethene, propene.
Butadiene, benzene, acetaldehyde not as well predicted
Linearity not always perfect

	n-Dodecane/m-Xylene	n-Dodecane/MCH	Spicer (JP-5/CFM-56/idle)	Aerodyne (AAFEX/JP-8)
CH4	0.36	0.29	0.43	-
C2H4	3.31	4.68	2.69	1.33
C3H6	0.58	0.55	0.79	0.51
C6H6	0.12	0.00	0.32	0.16
C4H6	0.03	0.10	0.30	-
CH3CHO	0.07	0.09	0.47	0.36

Uncertainties in scaling factors needs determination

- particularly large for propene

Summary of Simulation Conditions that Yielded Trend Data

One scenario: rapid quenching of rich pockets to very lean conditions

Critical conditions:

- Fuel rich phi: 1.6 to 2.2
- Quench residence time – 2.2 to 12 microseconds!
- Final phi - 0.1 to 0.2

Typical quench times:

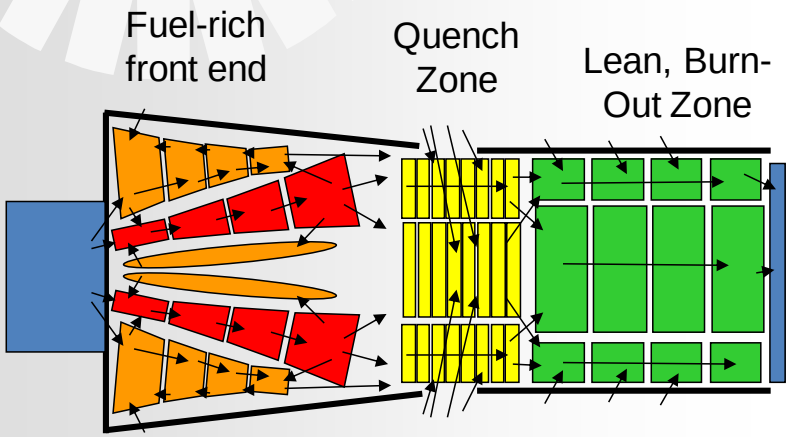
In traditional RQL burners > 0.1 milliseconds!

Possible mechanisms discussed at ESS/CI – October (Storrs, CT)

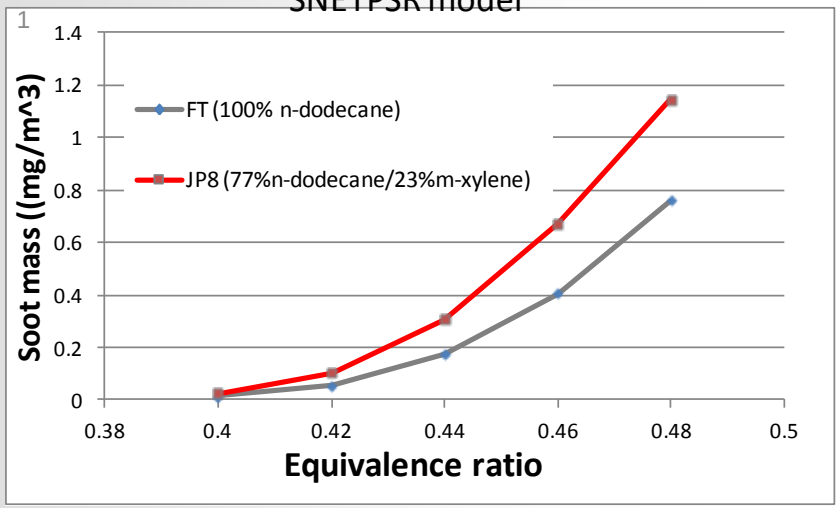
Simulation of PM emissions from RQL combustor

Reduced PM emissions with FT fuels

Full gas-phase and soot kinetics with aerosol dynamics model coupled into perfectly stirred reactor (PSR) network model

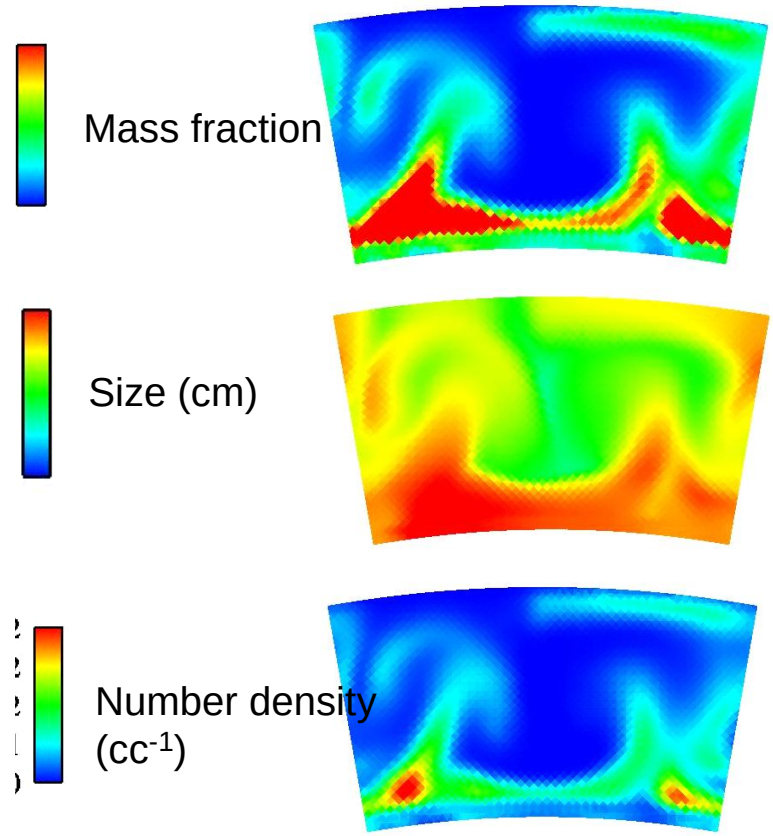


SNETPSR model



Predictions of mass, size, and number

Reduced-order model developed and installed into LES codes for predicting soot at combustor exit plane



Summary

- Coupling of chemistry amongst fuel molecules may be needed for simulation of extinction/LBO
- Physical effects are likely as/more important as chemical effects
- Kinetic models need to be accurate for phi variations
- Fuel rich chemistry (especially for aromatics) may need additional studies
- Preliminary coupled ignition model coupling kinetics/mixing/vaporization explains qualitative observations
- HC emissions fingerprint likely due to rapid quenching of reacting gas element

Recommendations/Needs – 2011

- Validated mechanisms that predict ignition and extinction
  - particularly aromatics and cycloalkanes
- Inclusion of ignition criteria for certification of alternative fuels
  - What should be the standard?
  - Incorporate physical effects?
- Soot models that predict fuel effects – (isoalkanes)
- Statistical methods for simulation of relative (physical/chemical) effects may be needed
- Review rich side chemistry, especially for aromatics

Thank You!!!!!

Acknowledgements:

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