Chemical Kinetic Modeling: A Status Report of Current Capabilities

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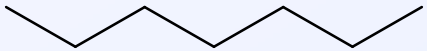
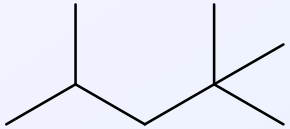
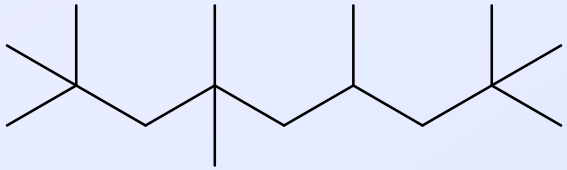
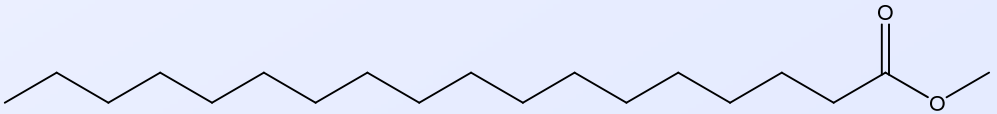
- DOE Office of Vehicle Technologies
  - Gurpreet Singh
  - Kevin Stork
- DOE Office of Basic Energy Sciences
  - Wade Sisk
- DOD Office of Naval Research

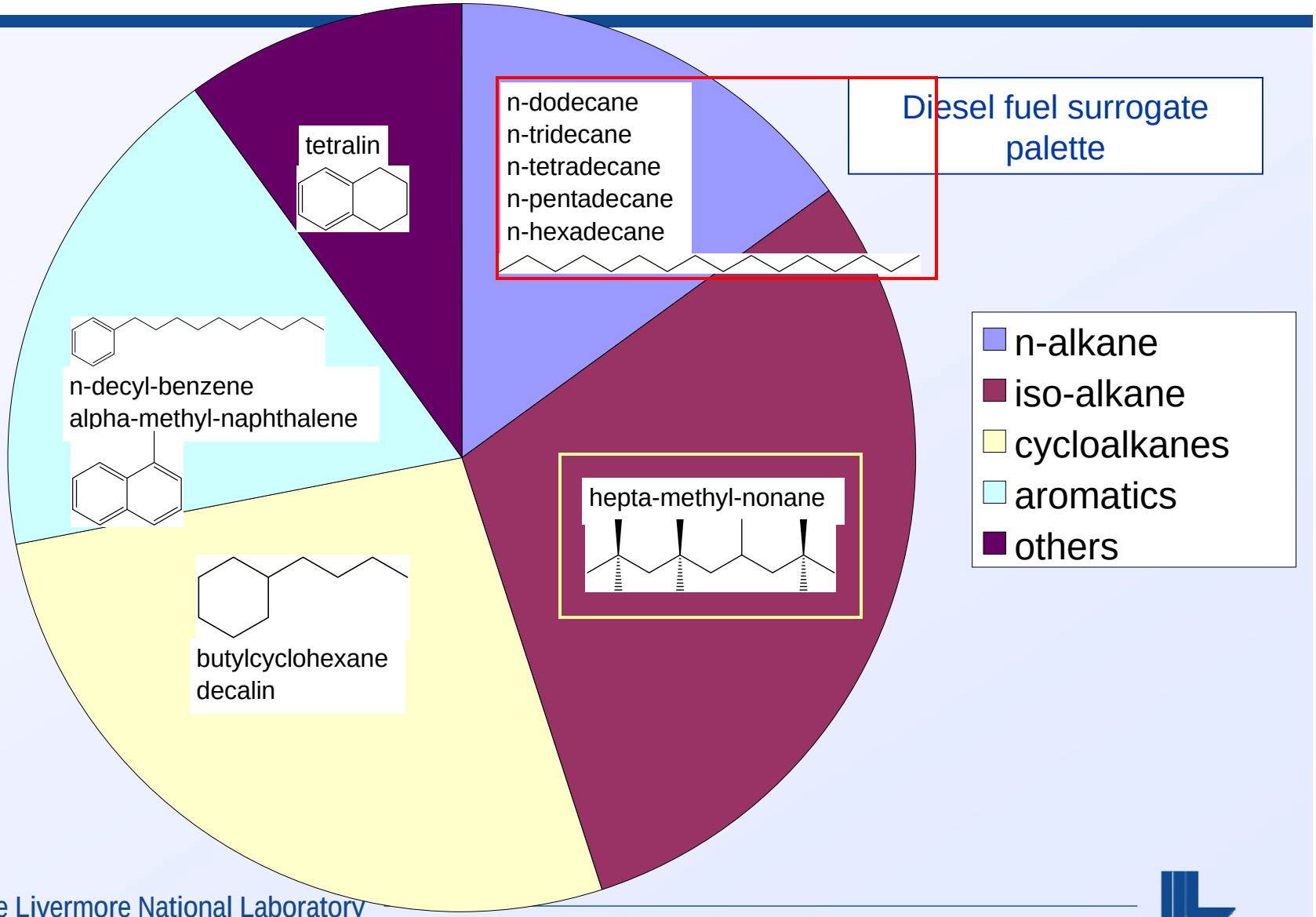
We develop chemical kinetic models, primarily for transportation fuels

- Gasoline
  - n-heptane 
  - iso-octane 
- Diesel
  - n-hexadecane 
  - 2,2,4,4,6,8,8-heptamethylnonane 
- Biodiesel 

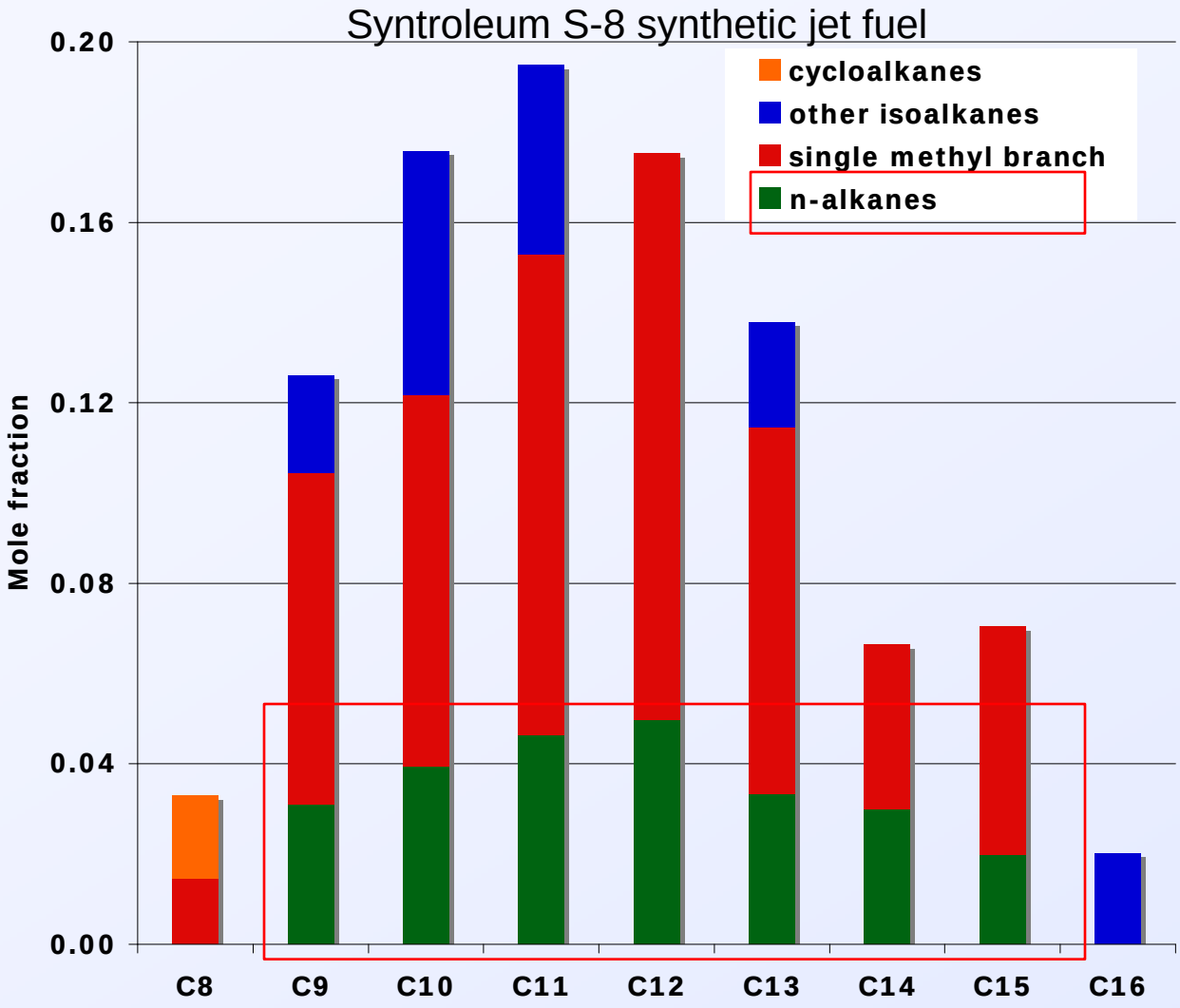
Concept of Primary Reference Fuel - PRF

- Octane in gasoline engines
  - Focus on knocking looks at the end of the combustion period
  - n-heptane ON = 0
  - iso-octane ON = 100
- Cetane in Diesel engines
  - Focus on ignition looks at the start of combustion
  - n-hexadecane CN = 100
  - iso-cetane CN = 15
- HCCI combustion has no explicit reference fuel that focuses on its unique engine history
- Note that all of these PRFs are n-alkanes or branched alkanes
- Each scale has an easily ignited PRF and a poorly ignited PRF
- ON and CN are engine-specific and fuel-specific
- Difference between Surrogate fuels and PRF

Development of chemical kinetic models for practical fuels presents challenges



We are developing chemical kinetic models for alternative fuels: Fischer-Tropsch fuels for jet engines



- FT analysis (NIST*)
  - 57% single methyl branch alkanes
  - 25% n-alkanes
  - 16% multiple branched alkanes
  - 2% cycloalkanes

*** Smith, B. L.; Bruno, T. J. *J. Propulsion* 2008, *24*, 618.**

New class of 2-methyl alkanes

C C C C C C … C C C n-alkanes

C
C C C C C C … C C C 2-methyl alkanes

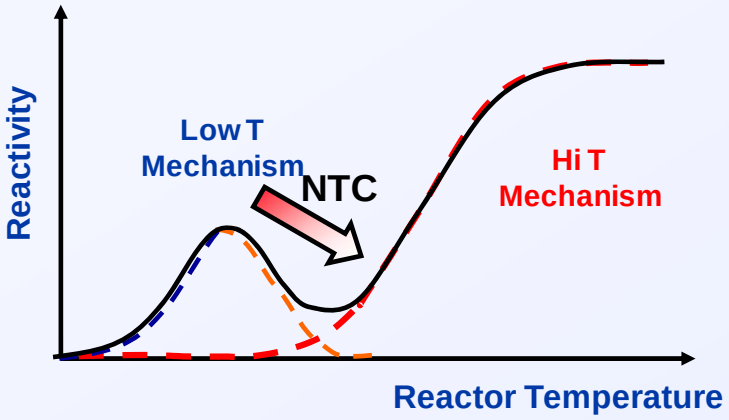
C
C C C C C C … C C C 3-methyl alkanes

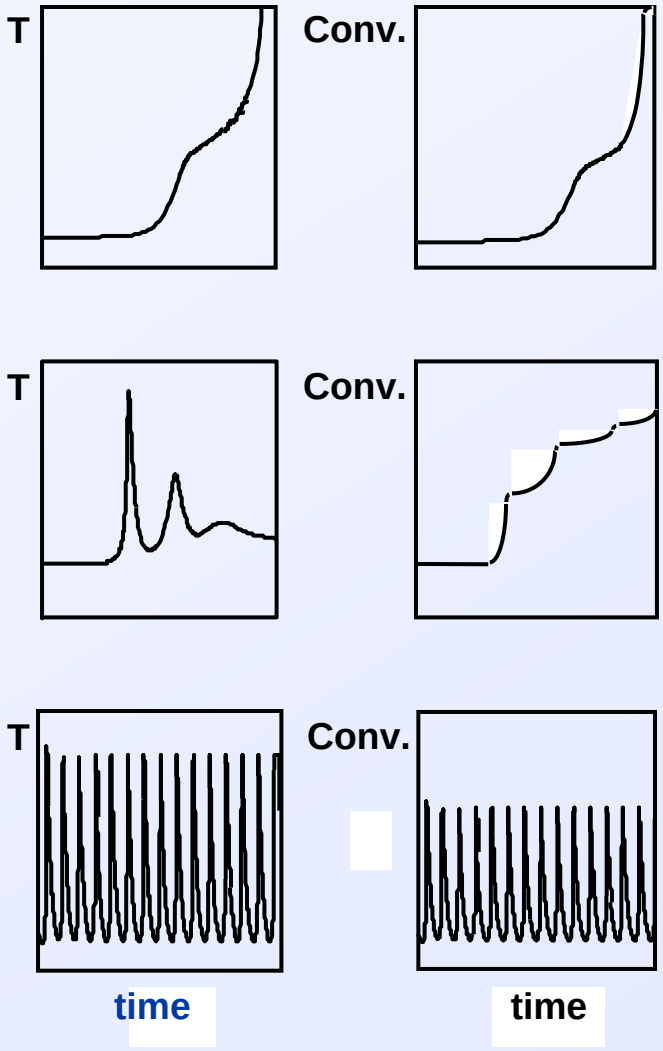
We expect to have these detailed mechanisms completed and available in a few months

All have chain lengths up to 20 C atoms

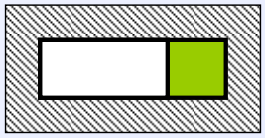
Alkanes oxidation in different reacting systems

Long Chain Alkanes



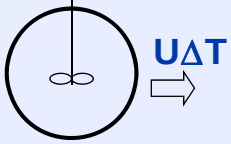


Closed Adiabatic



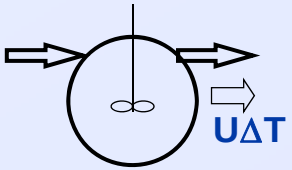
Closed

Non-Adiabatic

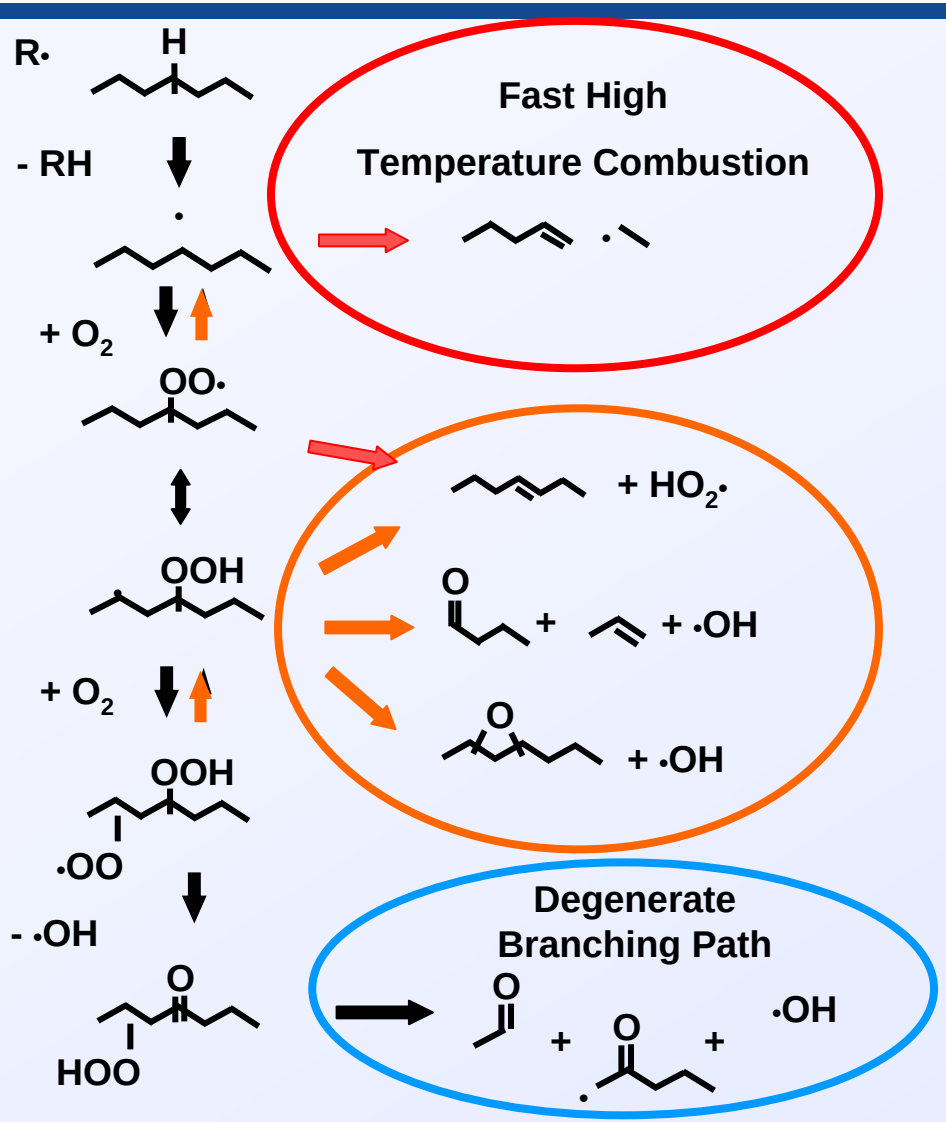


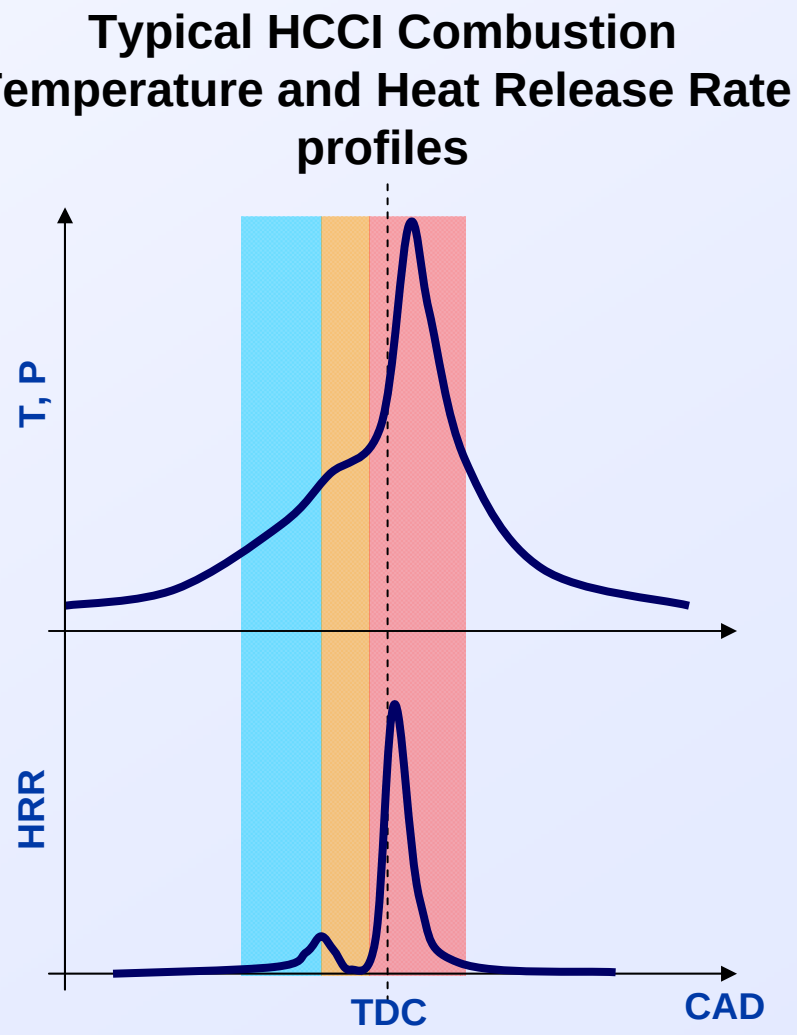
Open

Non-Adiabatic

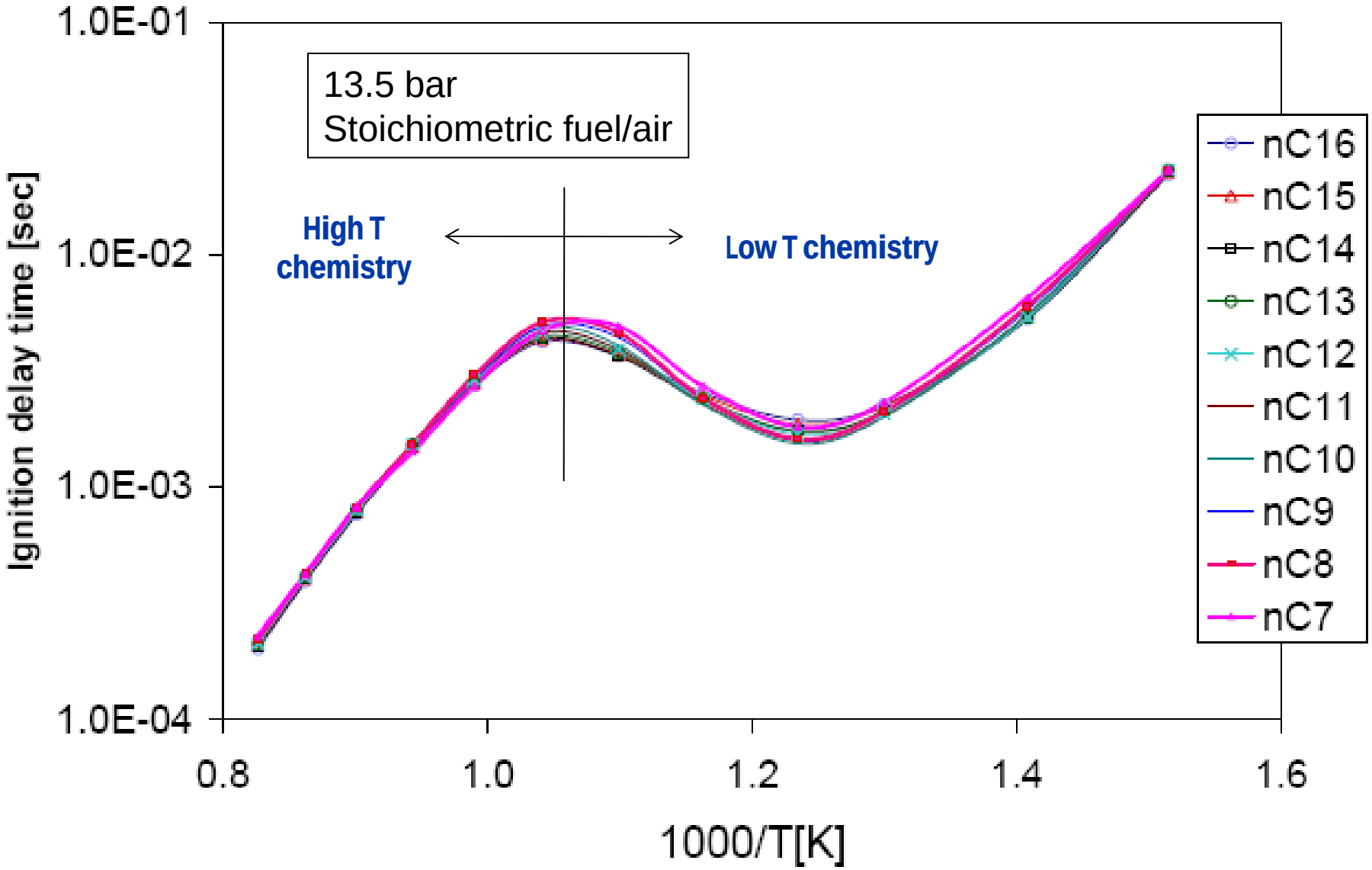


HCCI combustion kinetics: two Stage Fuels



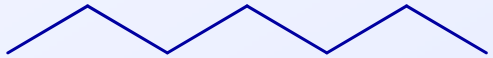


Low temperature kinetics responsible for NTC behavior



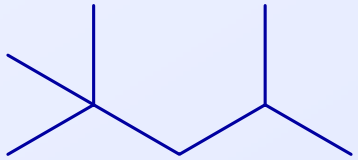
Recent accomplishments in chemical kinetic models for PRF fuels

- n-alkanes
  - Improved n-heptane model

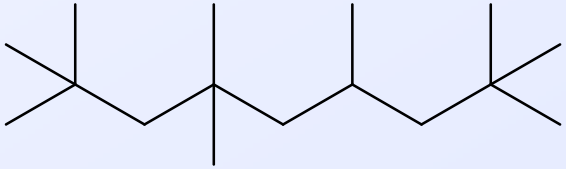


  - Recent model for C8 through C16 n-alkanes

- iso-alkanes:
  - Improved iso-octane model

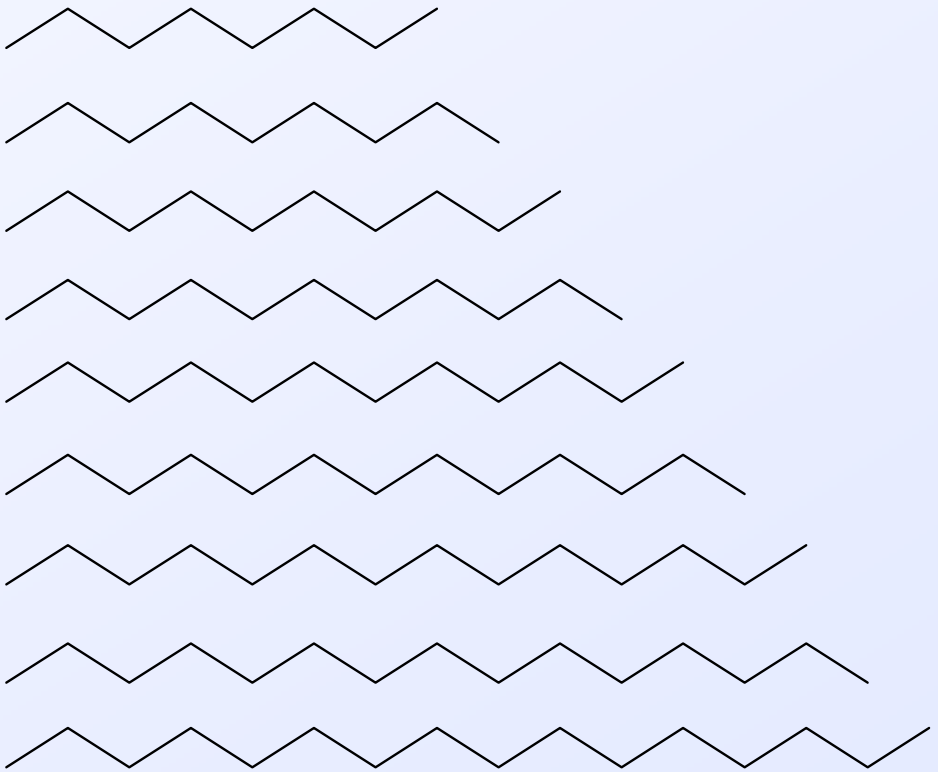


  - New 2,2,4,4,6,8,8-heptamethylnonane model



F-T fuels: We have extended our modeling capability for n-alkanes to cover a wide carbon range:

- n-octane (n-C8H18)
- n-nonane (n-C9H20)
- n-decane (n-C10H22)
- n-undecane (n-C11H24)
- n-dodecane (n-C12H26)
- n-tridecane (n-C13H28)
- n-tetradecane (n-C14H30)
- n-pentadecane (n-C15H32)
- n-hexadecane (n-C16H34)

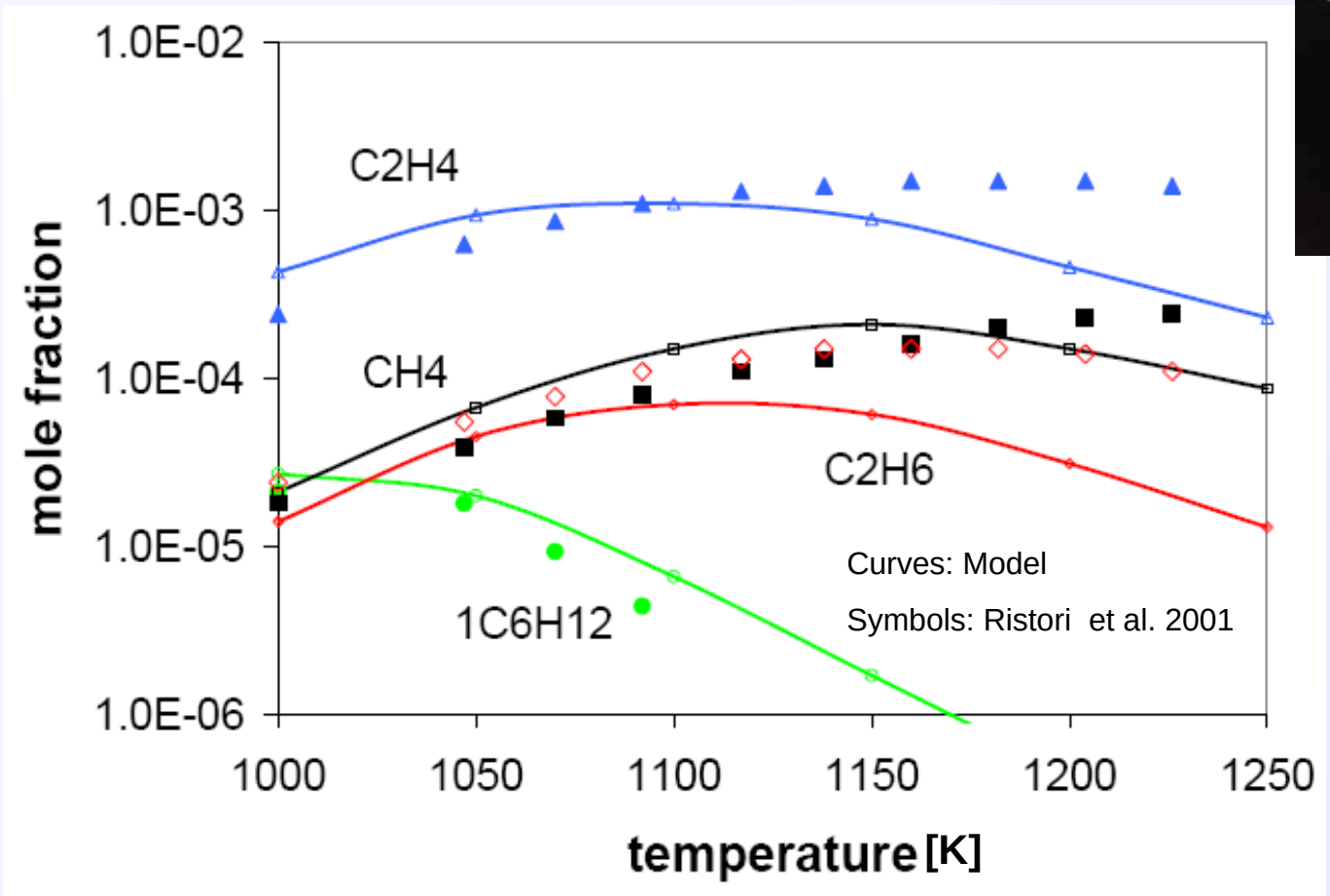


nC1-nC16 detailed chemistry model

- 2116 species
- 8130 reactions
- Low and high temperature chemistry => can use to investigate low temperature combustion strategies in diesel engines
- Same reaction rate rules as highly validated n-heptane mechanism
- Tailor the mechanism to fit specific fuels for computational efficiency

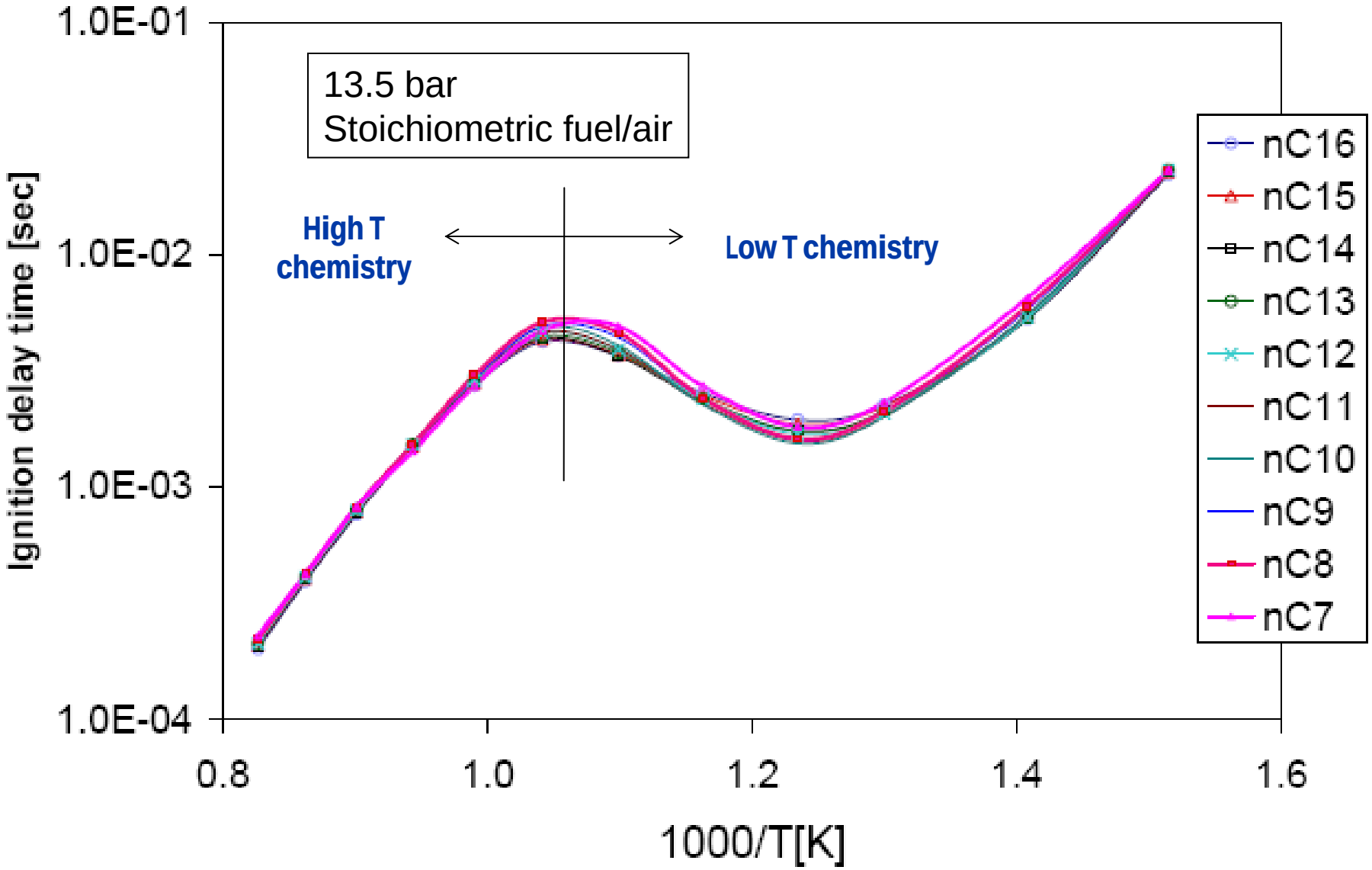
	$C_{16}H_{34}$	$C_{14}H_{30}$	$C_{12}H_{26}$	$C_{10}H_{22}$
Reactions	8130	6449	5030	3878
Species	2116	1668	1282	940

n-Hexadecane model behavior agrees reasonably well with experiments

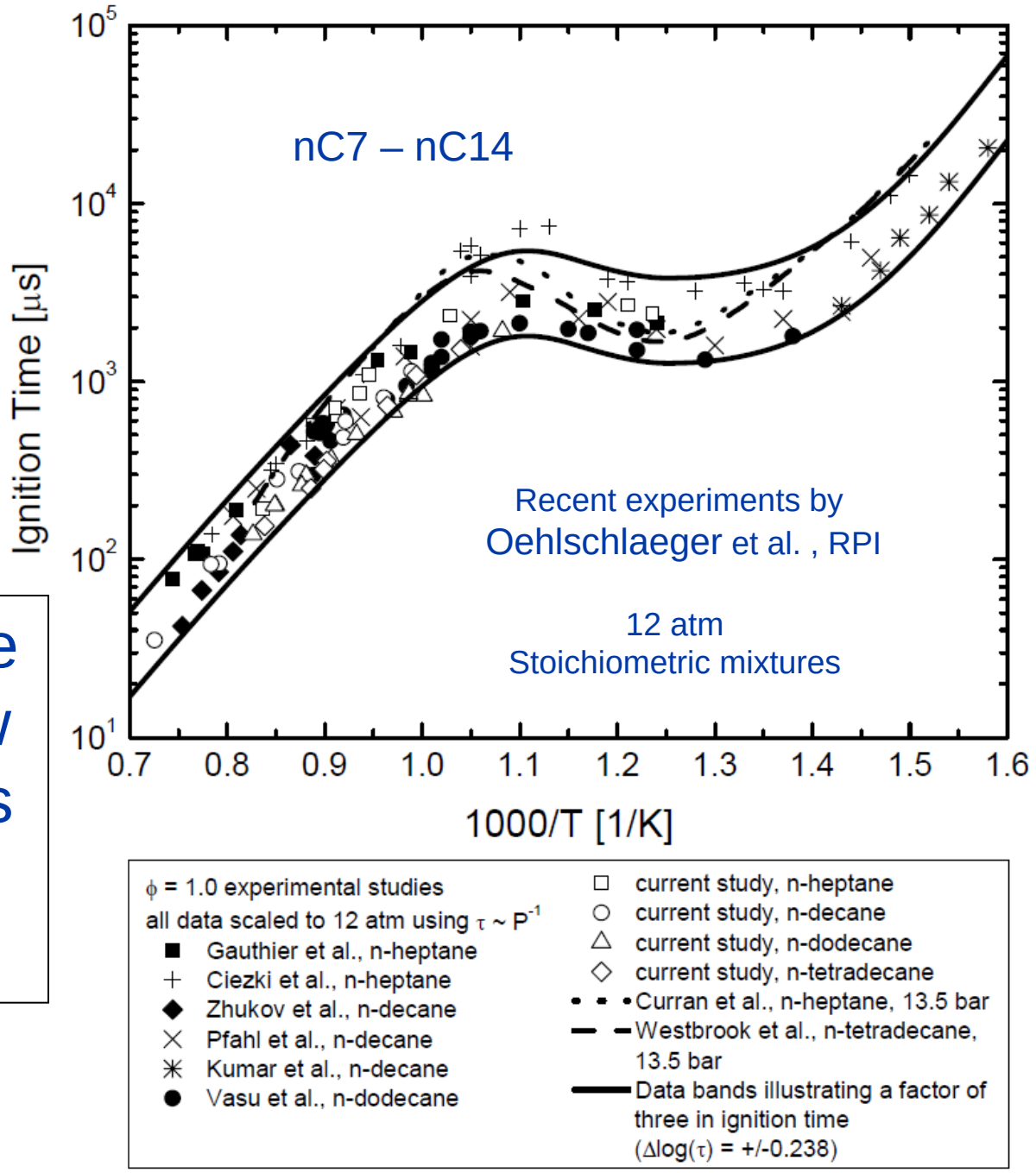


In stirred reactor at 1 atm, 1000-1250K, ϕ=1.5
70 ms residence time

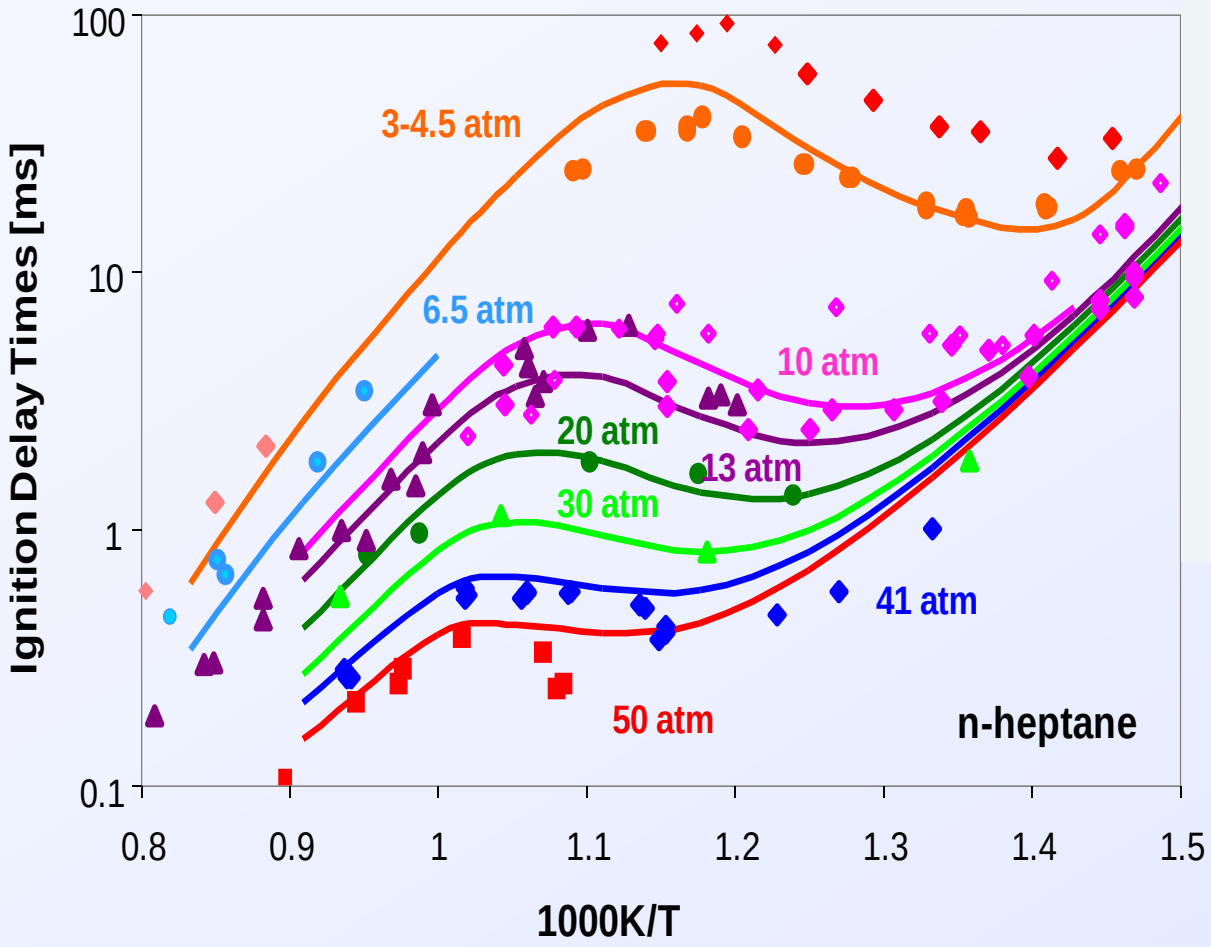
Predicted ignition behavior similar for C7-C16 n-alkanes



Recent shock tube experiments show all large n-alkanes ignite within a factor of 3



Improved component model for n-heptane simulates ignition over a wide temperature and pressure range:



P = 3 - 50 atm

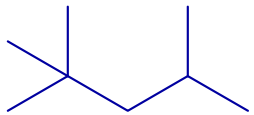
T = 650K - 1200K

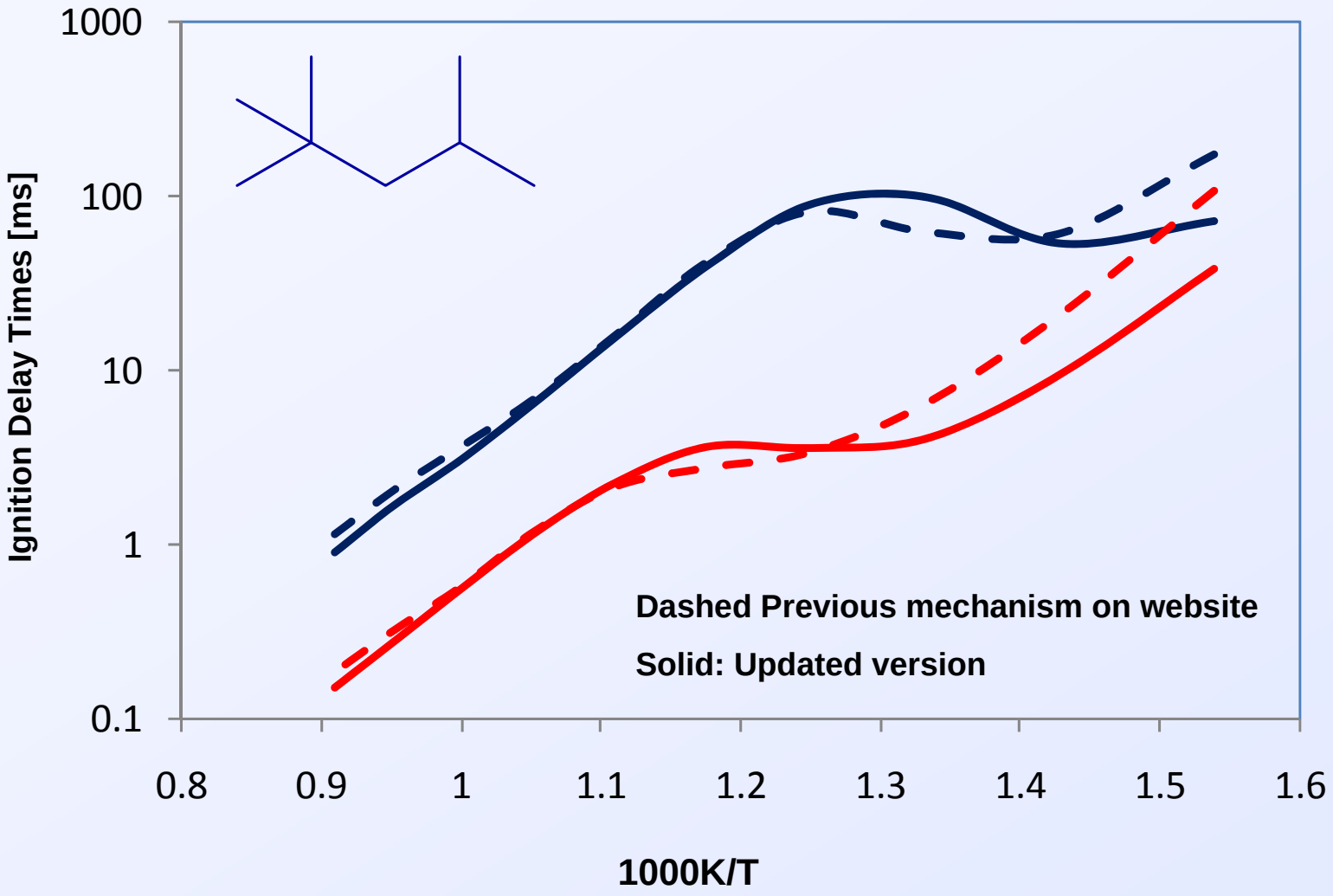
Φ = 1

Experimental data from shock tubes and rapid compression machines

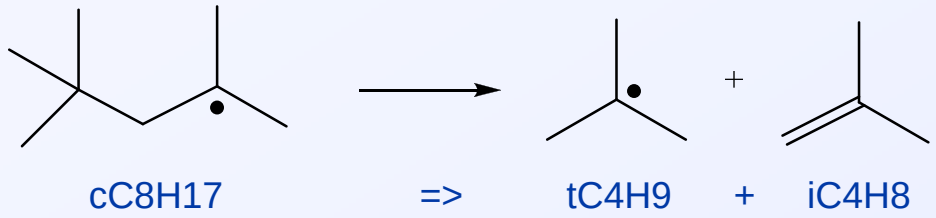
Experimental data: Minetti R., M. Carlier, M. Ribaucour, E. Therssen, L. R. Sochet (1995); H.K.Ciezki, G. Adomeit (1993); Gauthier B.M., D.F. Davidson, R.K. Hanson (2004); Minetti R., M. Carlier, M. Ribaucour, E. Therssen, L.R. Sochet (1996); K. Fieweger, R. Blumenthal, G. Adomeit (1997).

Improved component model to represent iso-alkanes in F-T fuels: iso-octane

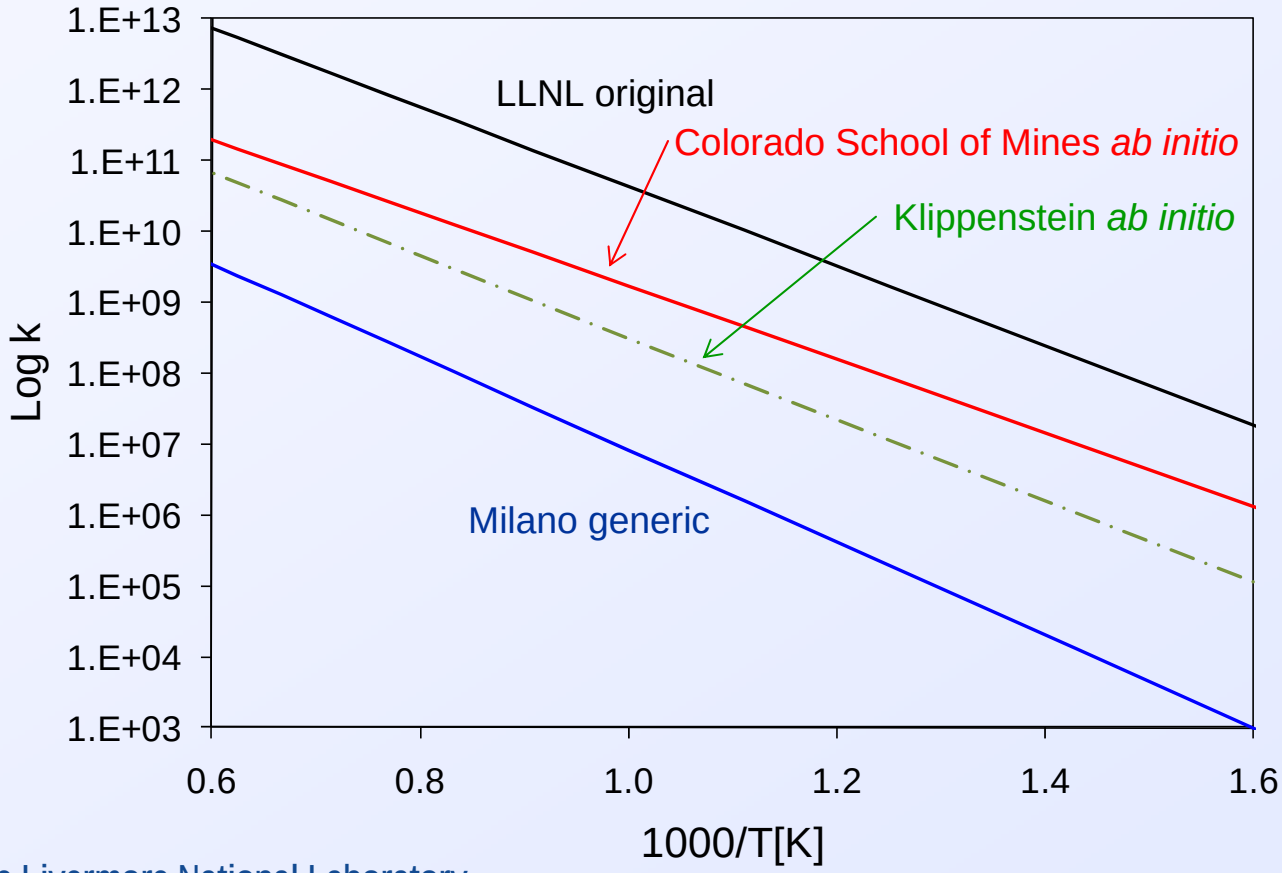




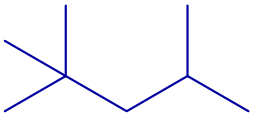
More accurate estimate for iso-octyl radical decomposition rate constant:



cC8H17 => tC4H9 + iC4H8



More accurately simulate ignition over a broad range of temperatures and pressure for iso-octane

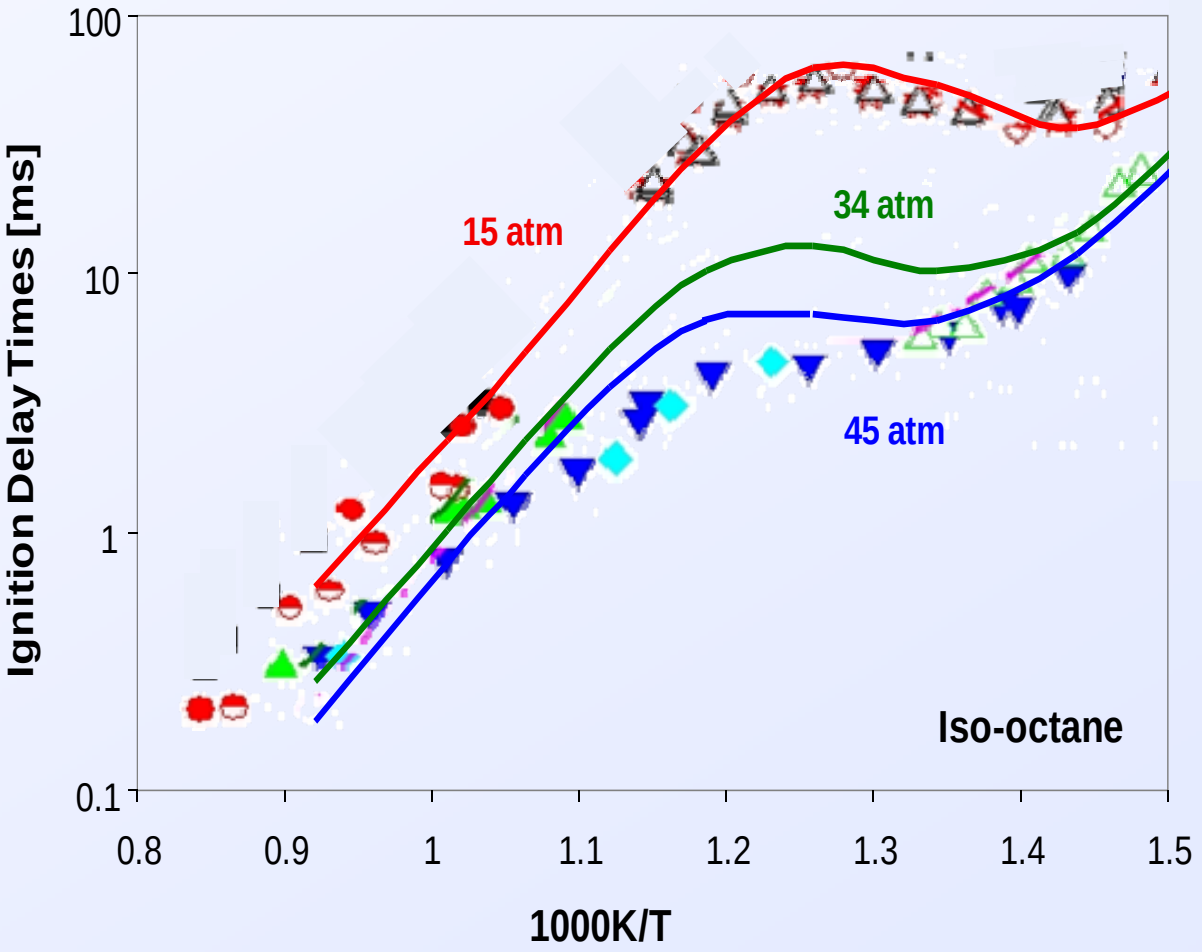


iso-octane:

P = 15 - 45 atm

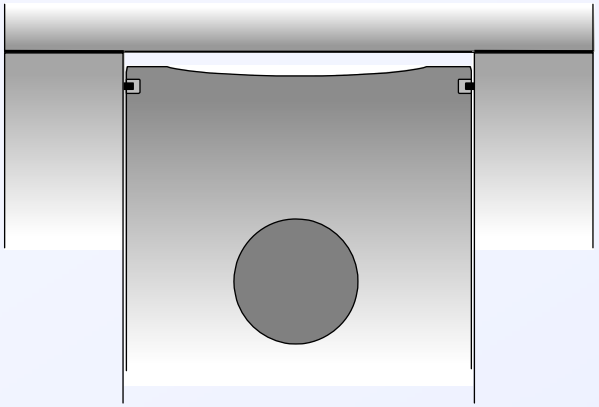
T = 650K - 1150K

Φ= *1*

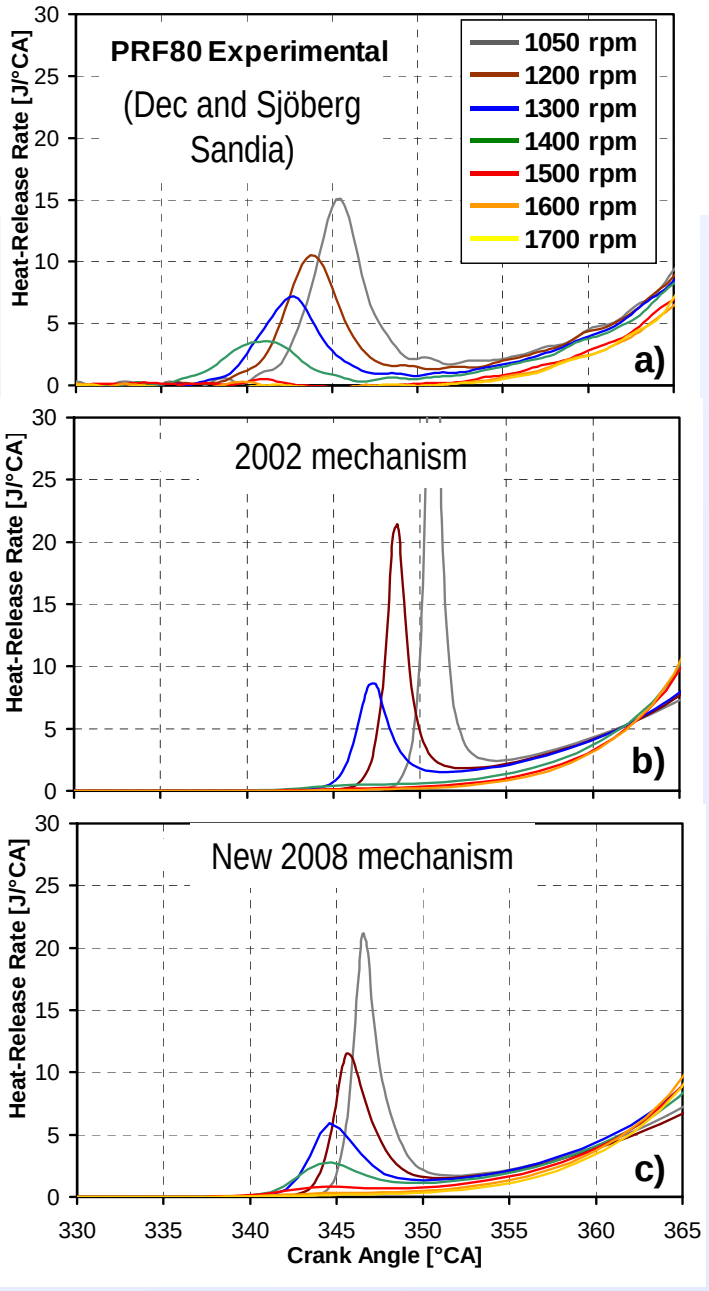


Experimental data:
Mittal G. and C. J. Sung, 2007; Minetti R., M. Carlier, M. Ribaucour, E. Therssen, L.R. Sochet, 1996; K. Fieweger, R. Blumenthal, G. Adomeit , 1997.

HCCI engine results with combined n-heptane/iso-octane mechanism:



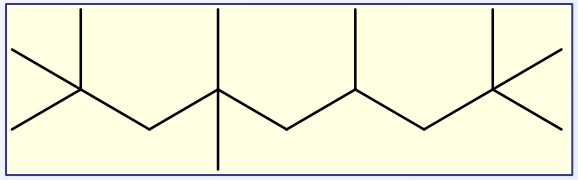
Better simulation of heat release rate



PRF80 fueling

(80% iso-octane and 20% n-heptane)

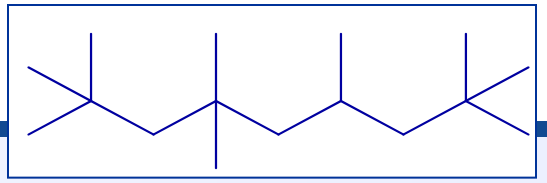
Development of new detailed chemical kinetic model to represent a large iso-alkane: heptamethylnonane (HMN)

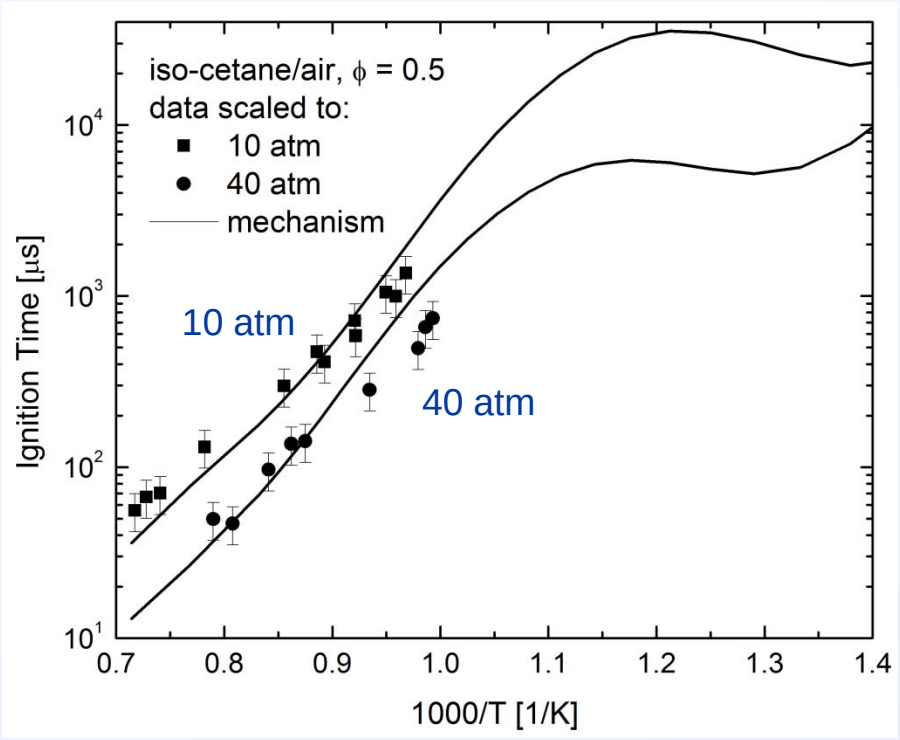


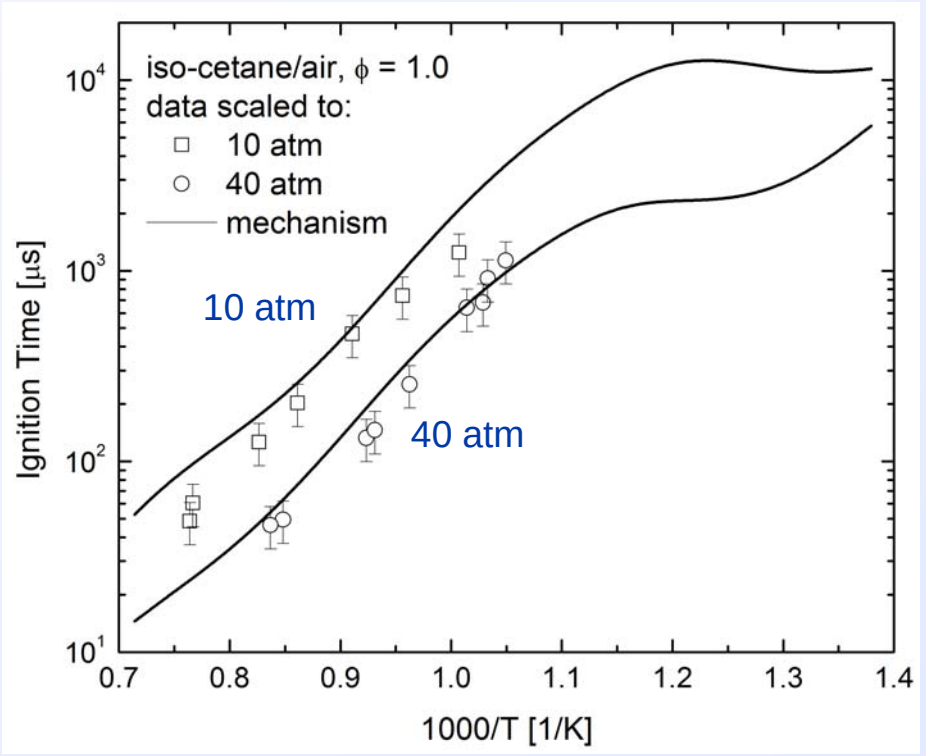
2,2,4,4,6,8,8 heptamethylnonane

- Primary reference fuel for diesel
- Based on reaction rate rules of iso-octane mechanism
- Includes low and high temperature reactions
- 1114 species
- 4468 reactions

Recent experimental results show good agreement with modeling for HMN

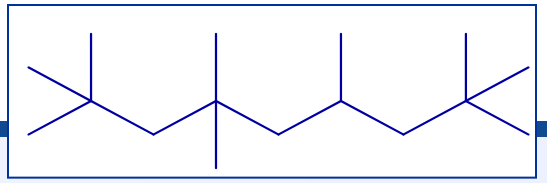


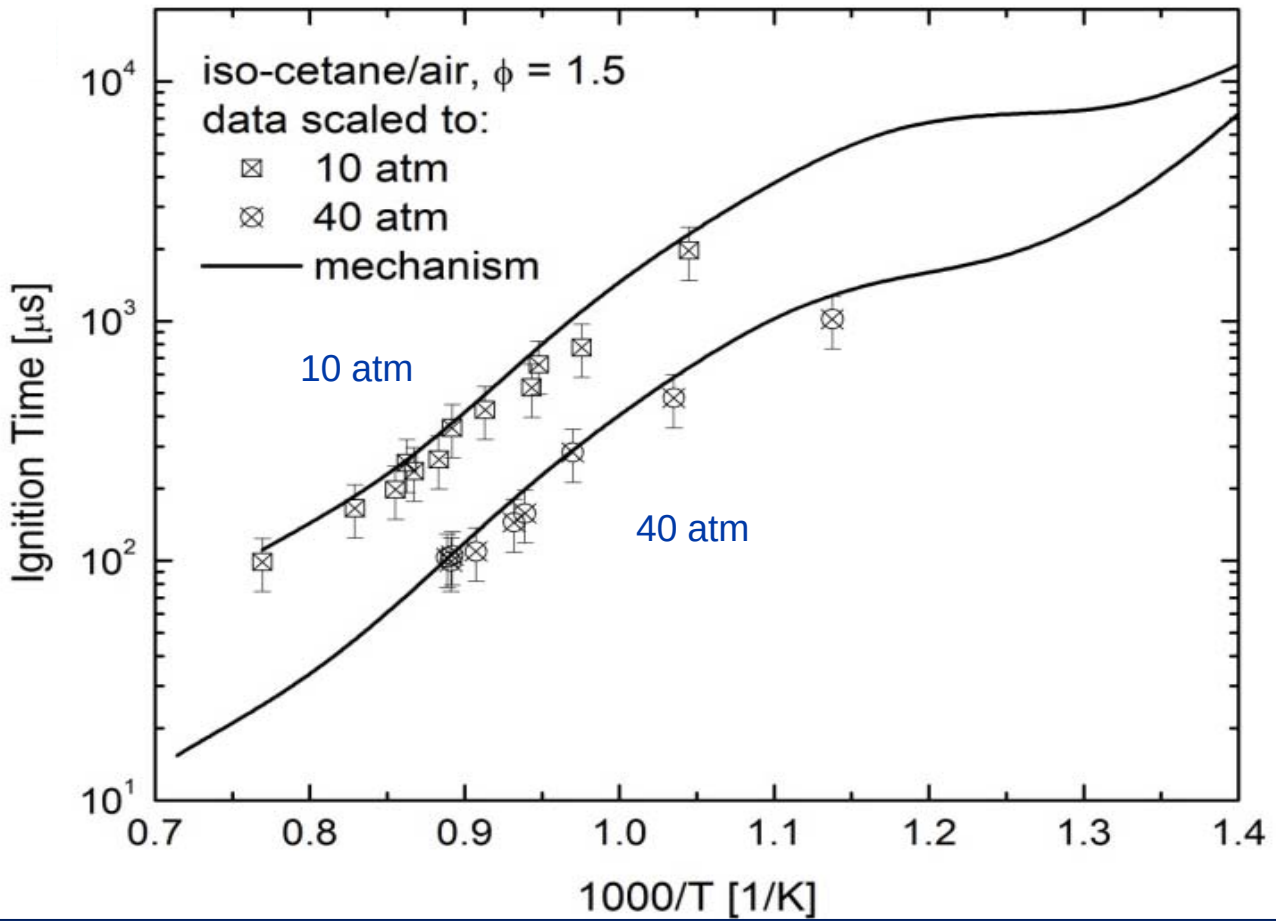




Oehlschlaeger, Steinberg, Westbrook and Pitz, Combustion Flame, 2009

Recent experimental results show good agreement with modeling for HMN

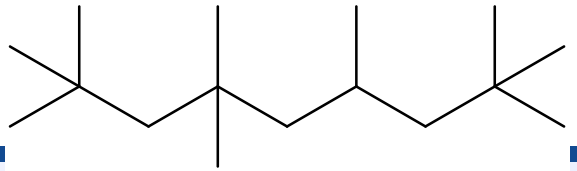


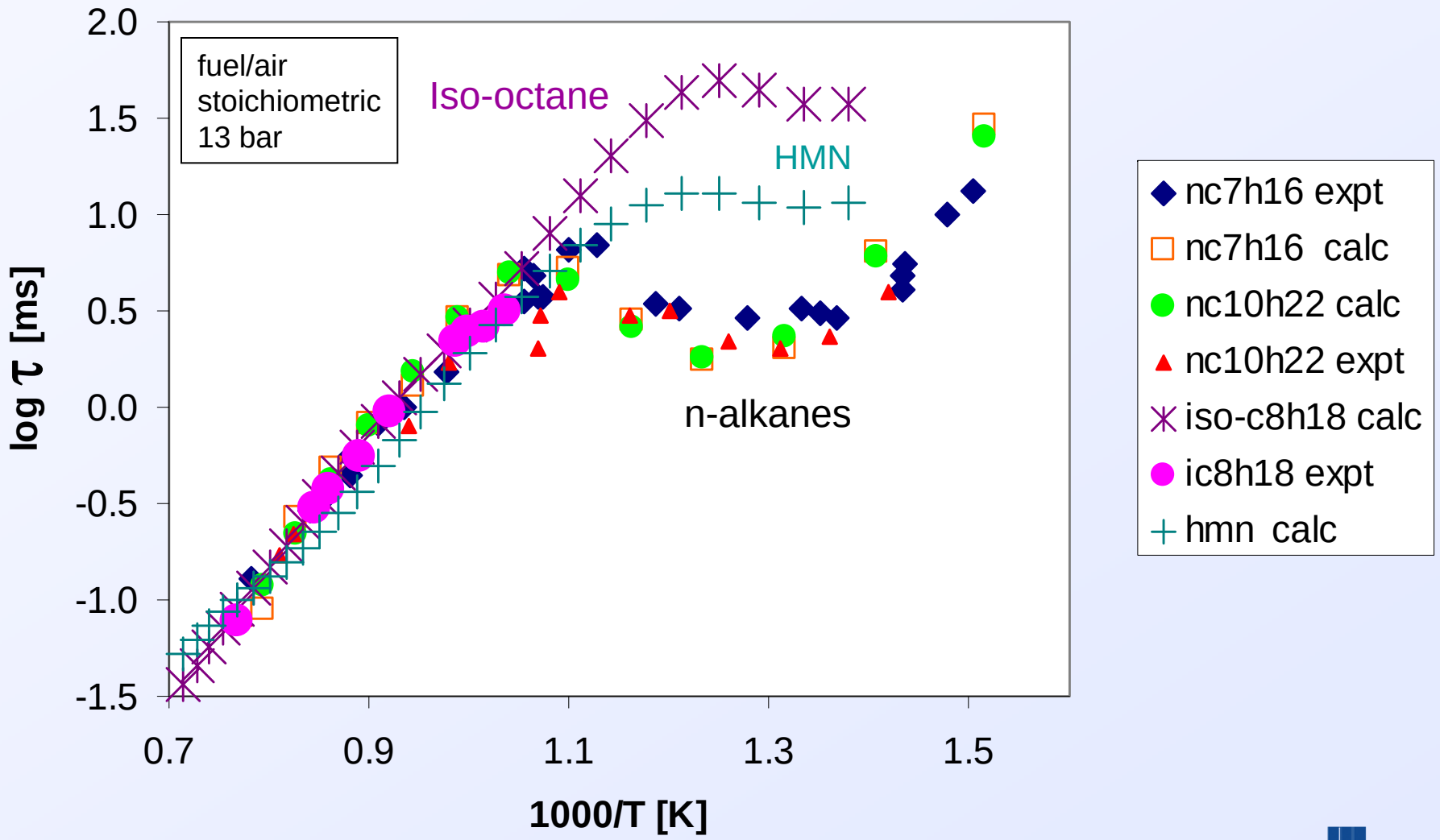


Oehlschlaeger, Steinberg, Westbrook and Pitz, Combustion Flame, 2009

HMN ignition results at 13 bar:

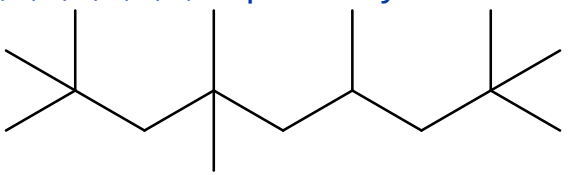
2,2,4,4,6,8,8, heptamethylnonane

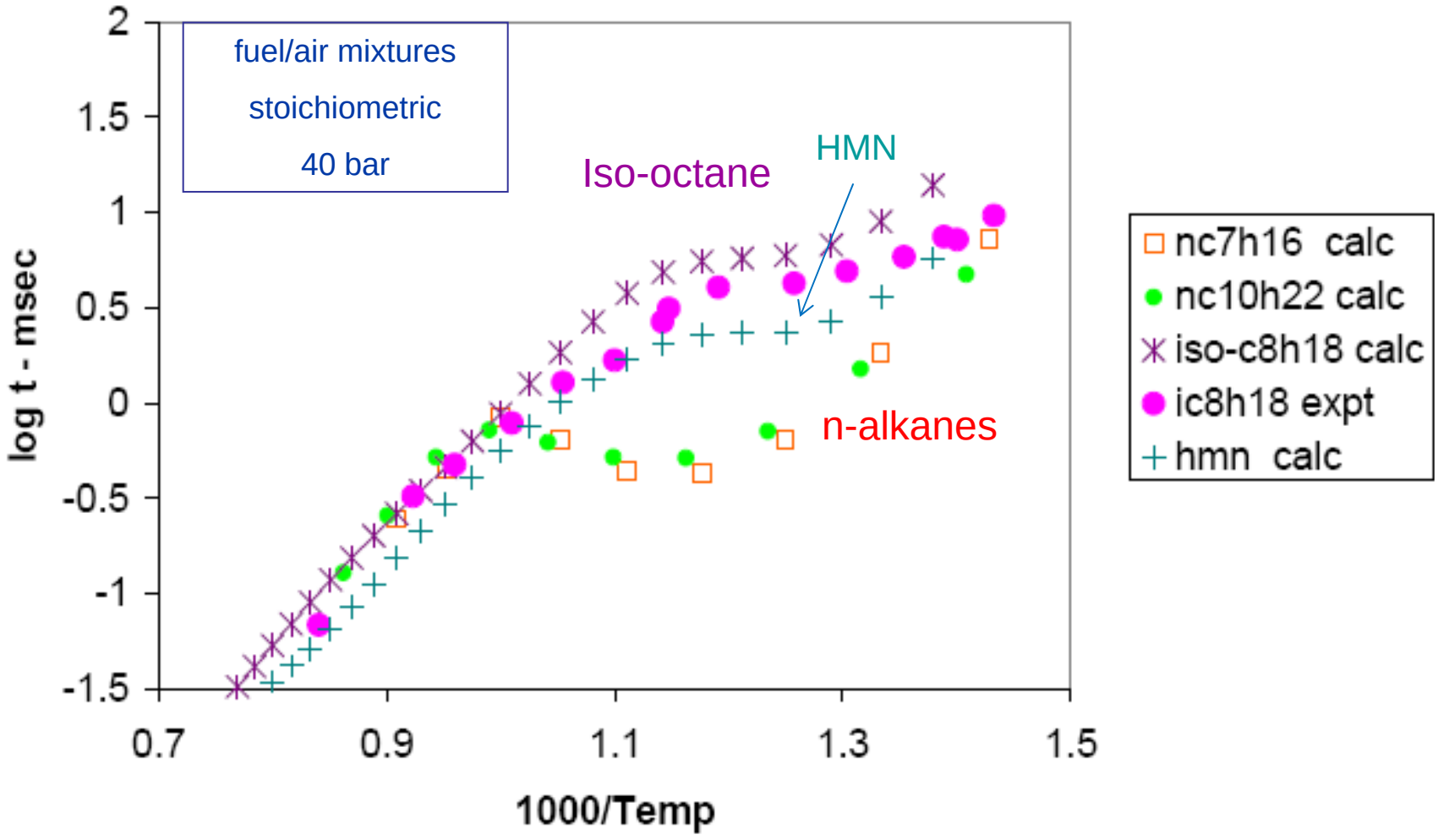




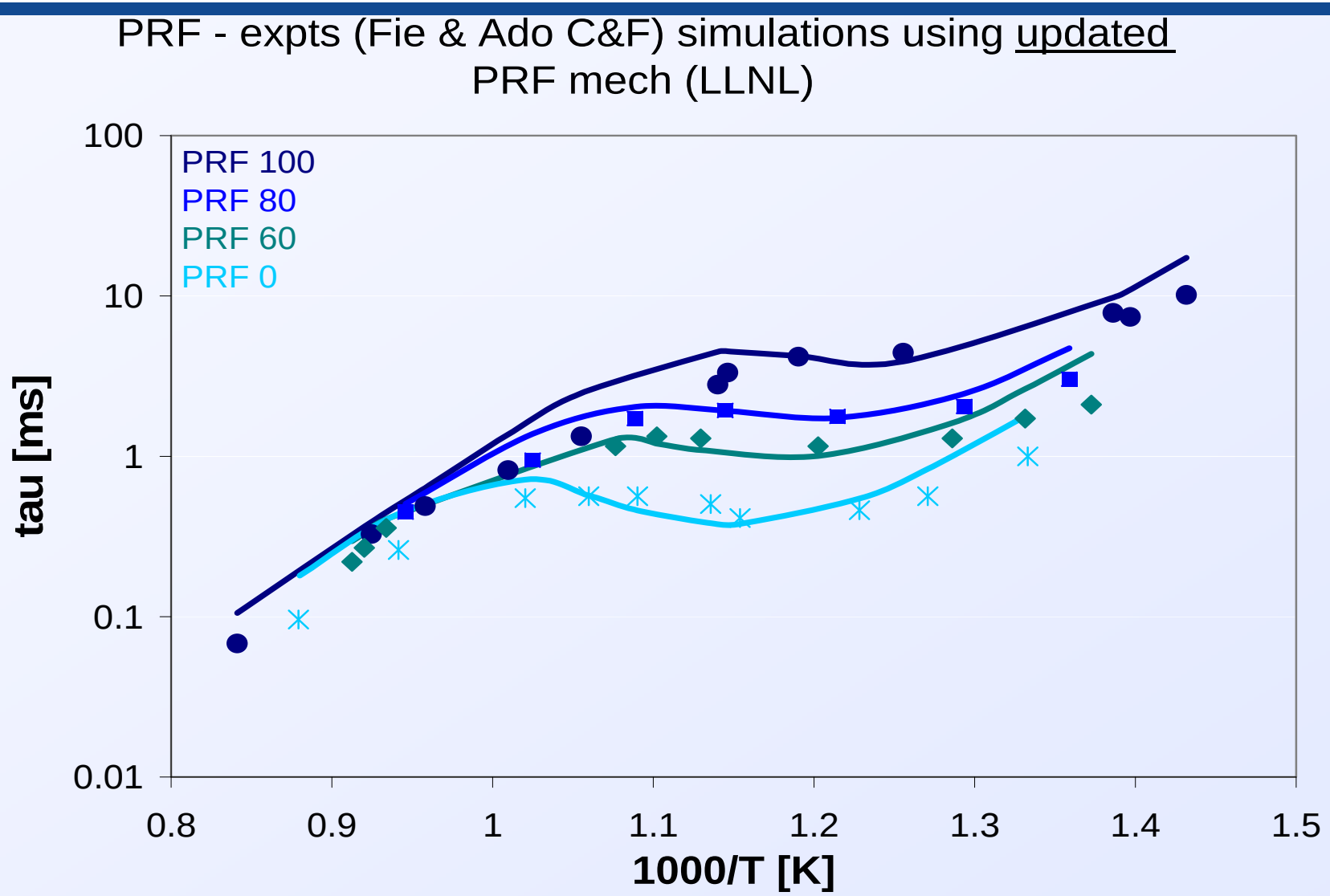
HMN ignition results at 40 bar:

2,2,4,4,6,8,8, heptamethylnonane





Ignition of Gasoline PRF Mixtures

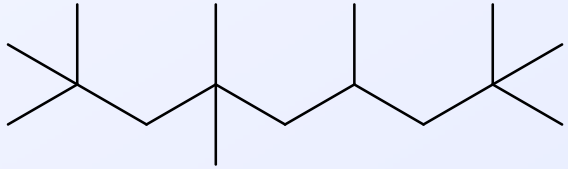


Have assembled primary reference fuel mechanism for diesel fuel

- Diesel PRF:
  - n-cetane

(n-hexadecane)

  - iso-cetane



(2,2,4,4,6,8,8-heptamethylnonane)

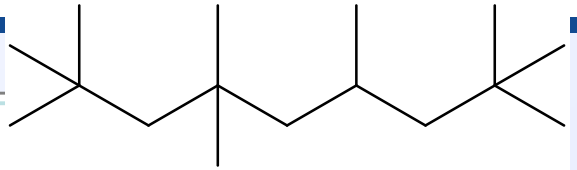
- PRF for Diesel mechanism:
  - 2,837 species
  - 10,719 reactions

Methyl stearate

PRF Ignition results at 13 bar:

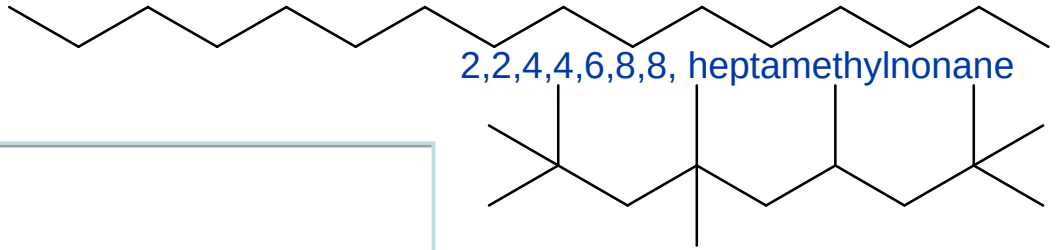
n-hexadecane

2,2,4,4,6,8,8, heptamethylnonane



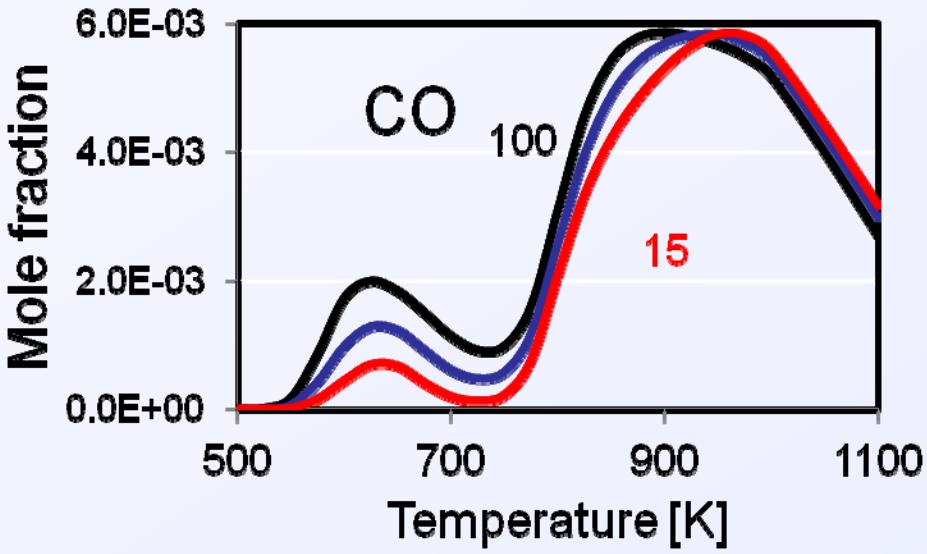
PRF Ignition results at 40 bar:

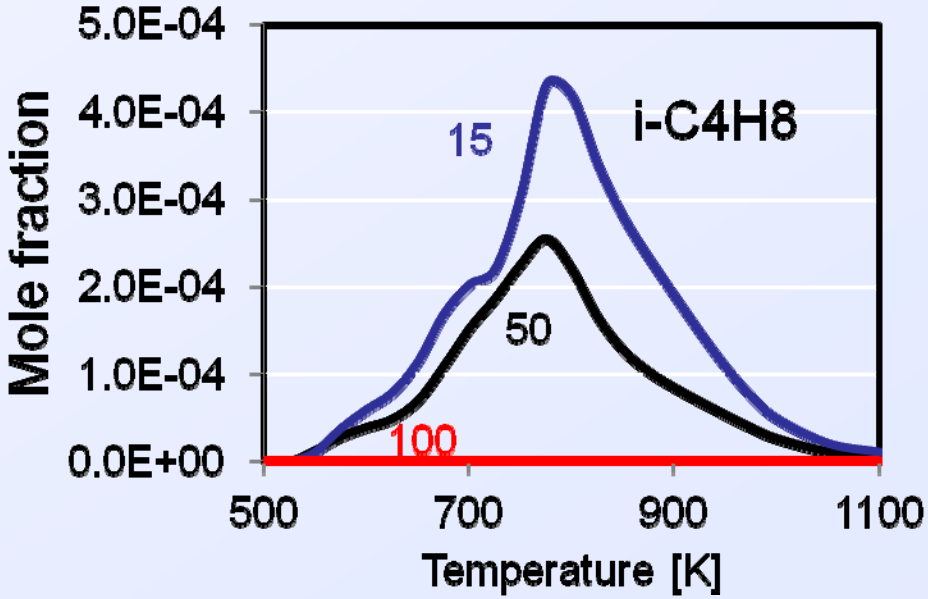
n-hexadecane



2,2,4,4,6,8,8, heptamethylnonane

CN has biggest effect at low temperatures

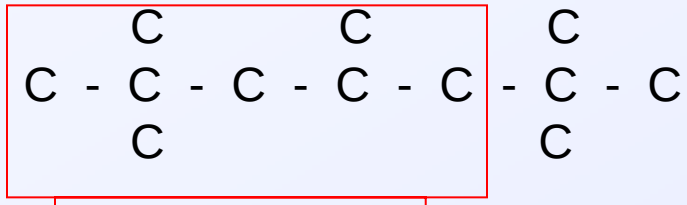




Expanding the palette for large iso-alkanes: iso-dodecane ($C_{12}H_{26}$)

- Lightly branched, large iso-alkanes are not available from suppliers

2,2,4,6,6-pentamethyl heptane



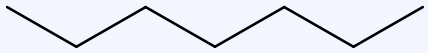
isomer A

2,3,4,5,6-pentamethyl heptane

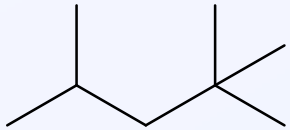
isomer B

- Isomer A has only one tertiary H-atom. Has many of the structural features of iso-octane and heptamethylnonane
- Isomer B is quite different: has many tertiary H-atoms.

Need to reduce chemical kinetic models to couple them to multi-dimensional CFD codes to model combustion in engines

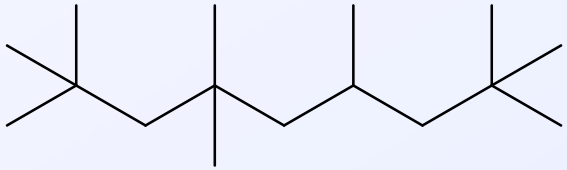


n-heptane



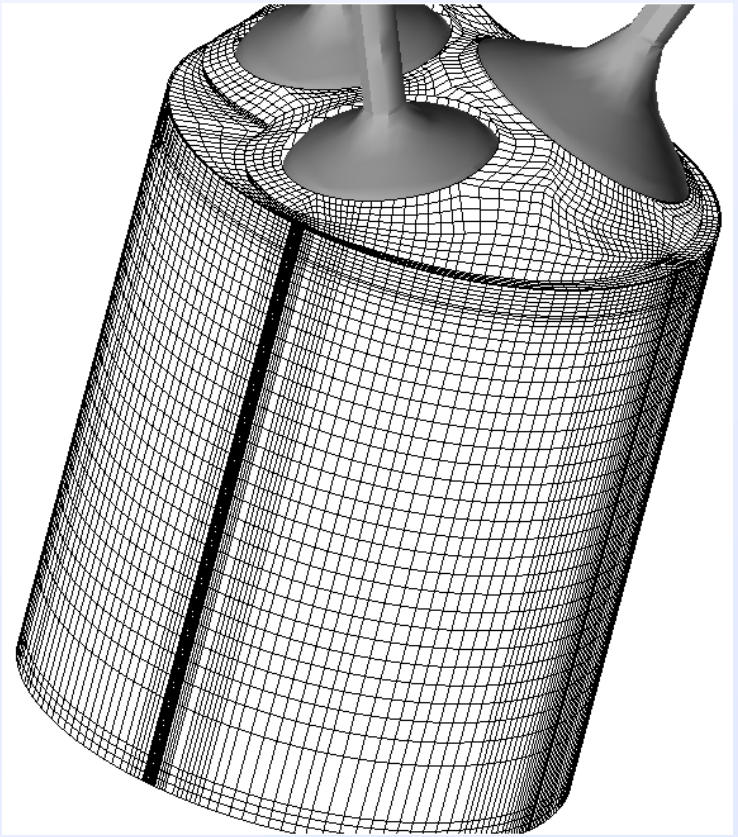
iso-octane

n-hexadecane



2,2,4,4,6,8,8 heptamethylnonane

Chemical kinetic models for primary reference fuels for gasoline and diesel



We collaborate with others to reduce our models for use in reacting flow codes

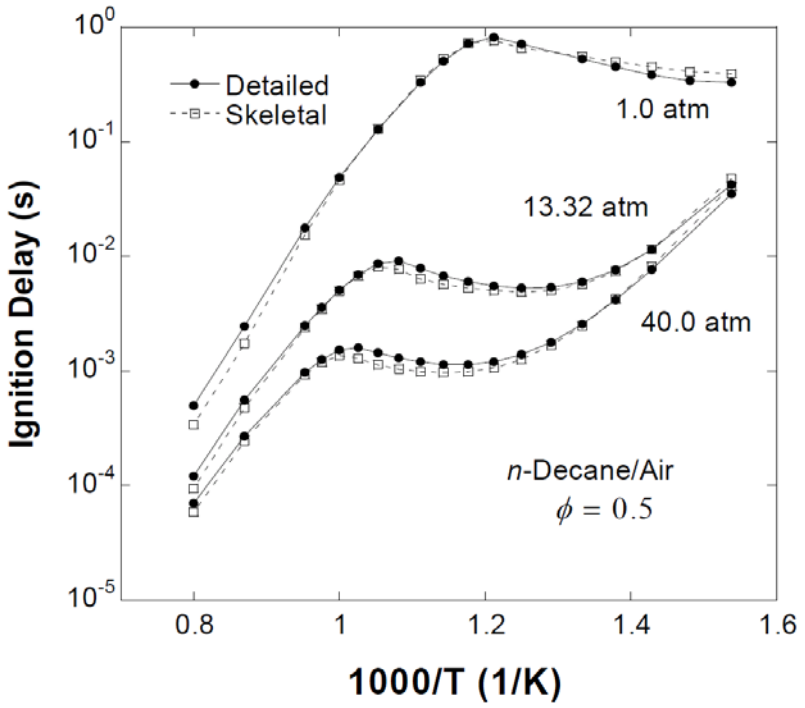
n-decane

940 species
3887 reactions

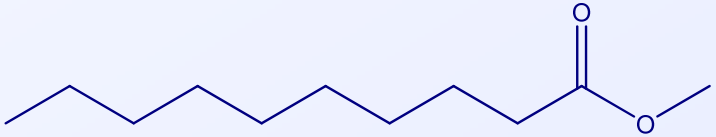
⇨

211 species
794 reactions

Niemeyer, Raju and Sung, 2009



Methyl-decanoate, biodiesel surrogate

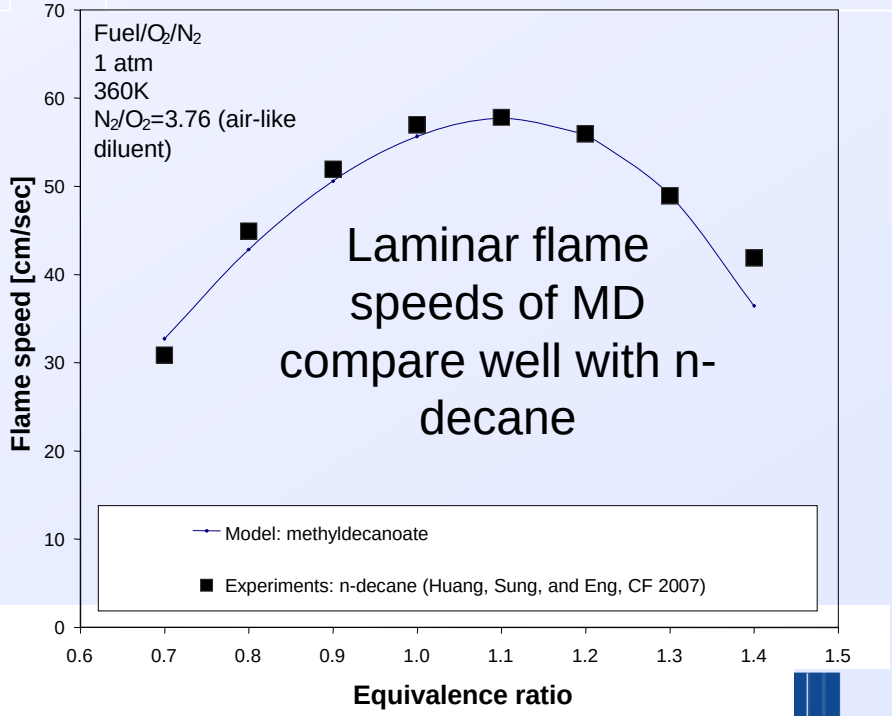


3036 species
8555 reactions

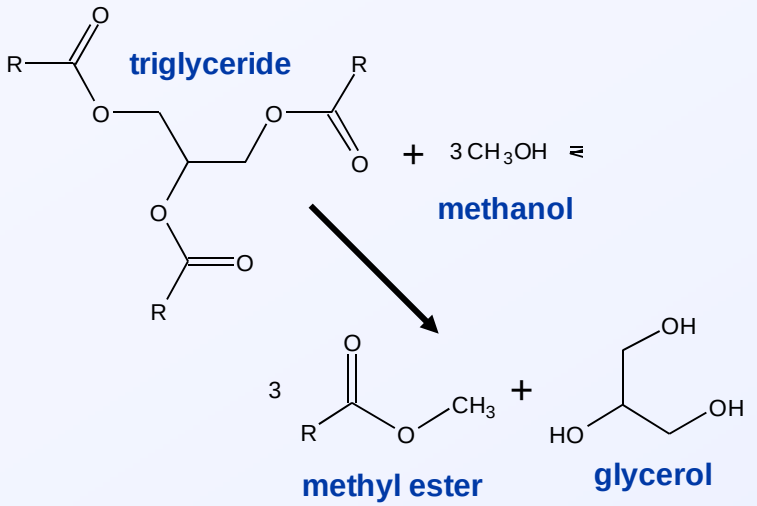
⇨

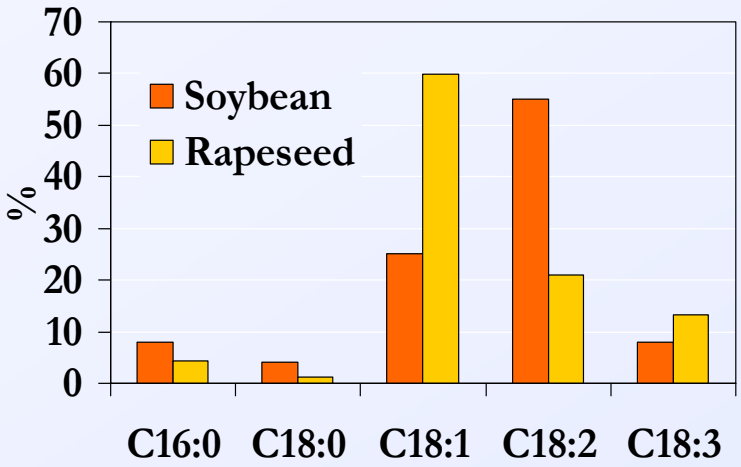
125 species
712 reactions

Tianfeng Lu and C. K. Law, 2009

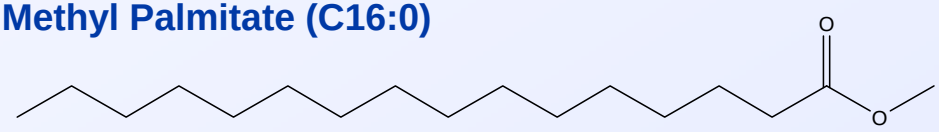


Composition of Biodiesels

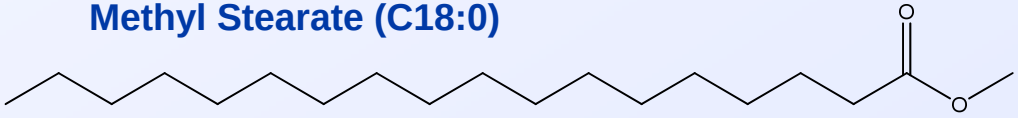




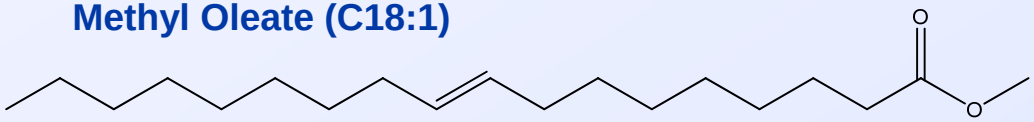
Methyl Palmitate (C16:0)



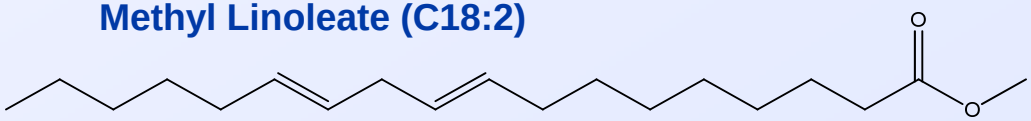
Methyl Stearate (C18:0)



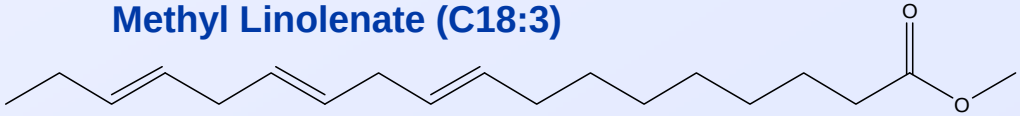
Methyl Oleate (C18:1)



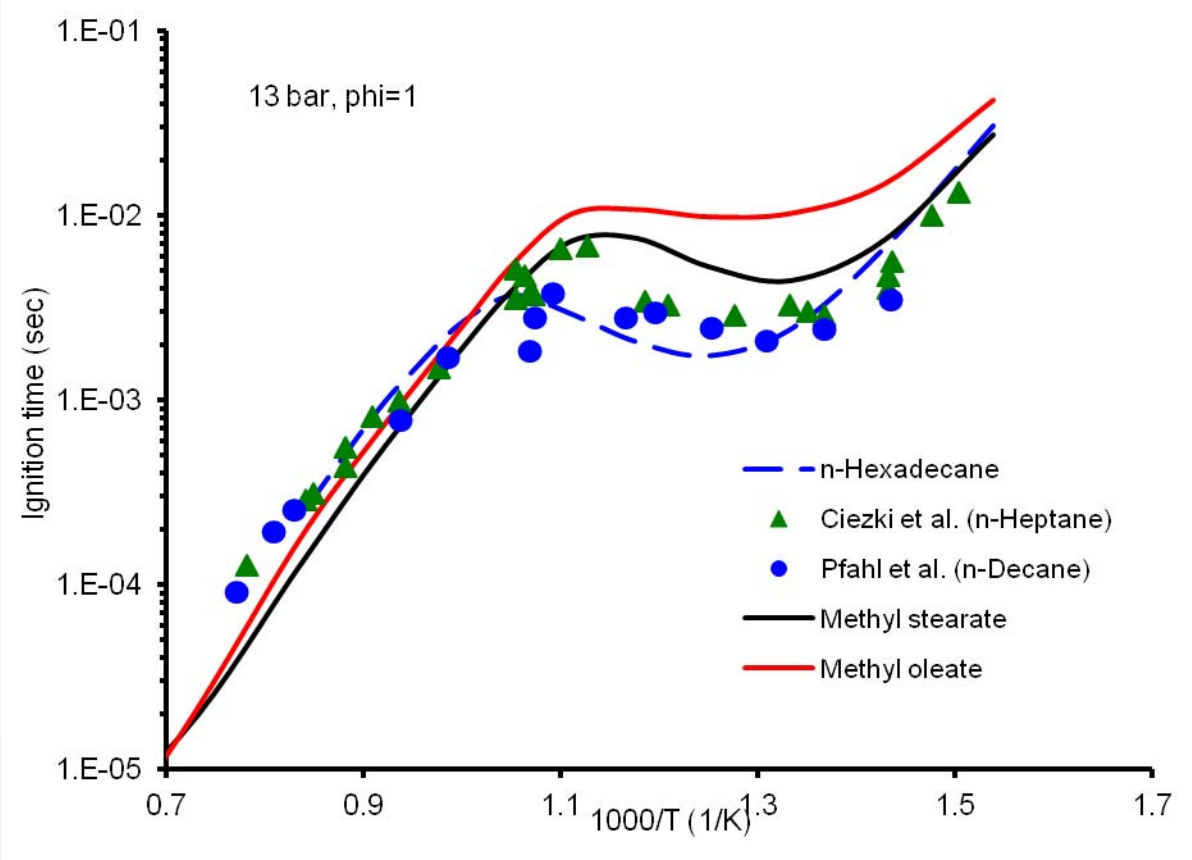
Methyl Linoleate (C18:2)



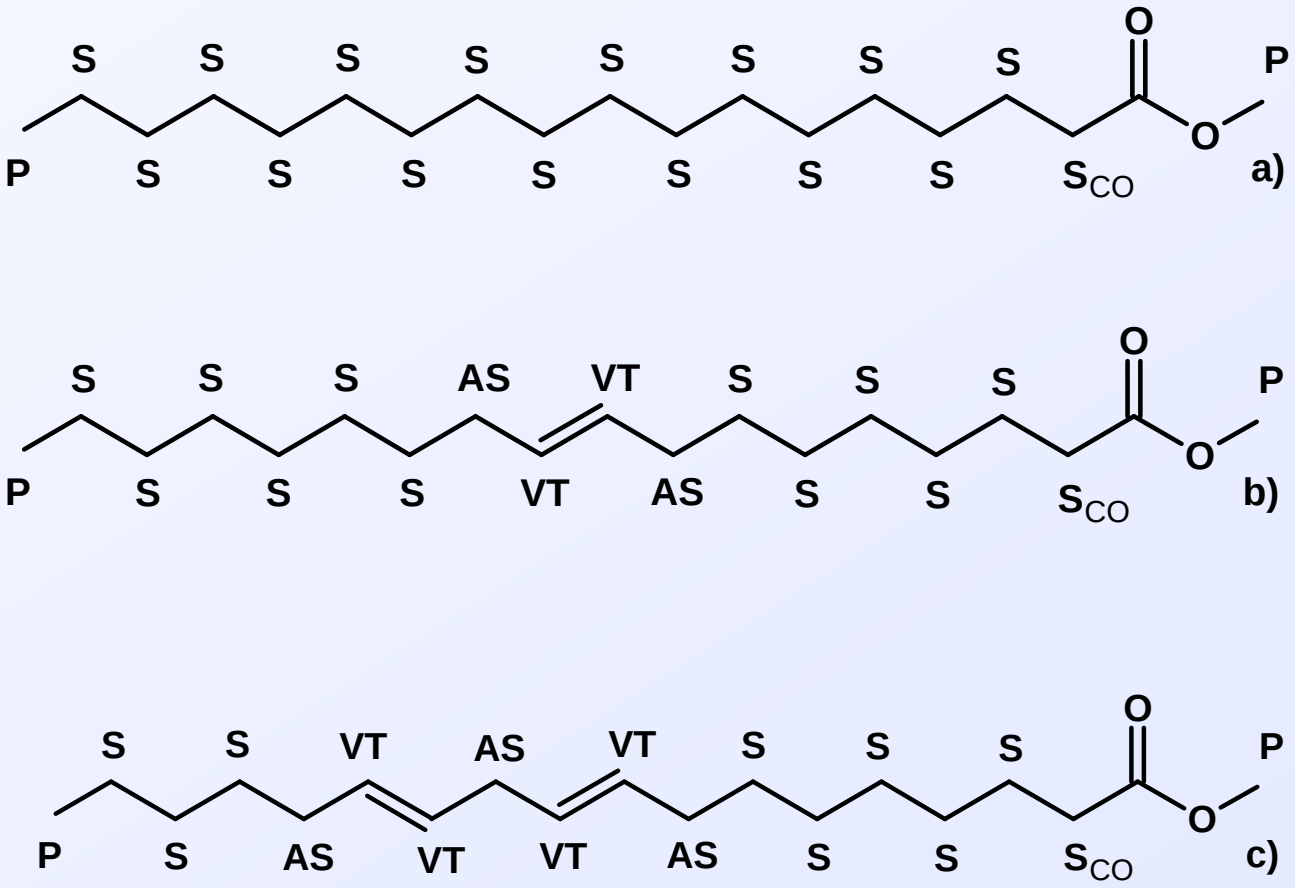
Methyl Linolenate (C18:3)



Methyl stearate is more reactive than methyl oleate in low T region

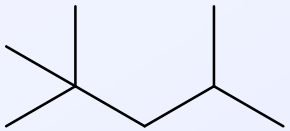


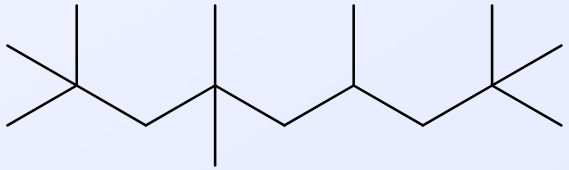
Double bonds reduce low T reactivity



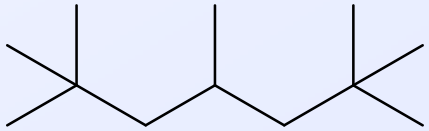
Summary

- Developed/improved fuel component models for transportation fuels:
  - n-alkanes:
    - n-heptane
    - C8 through C16
  - Iso-alkanes:
    - Iso-octane

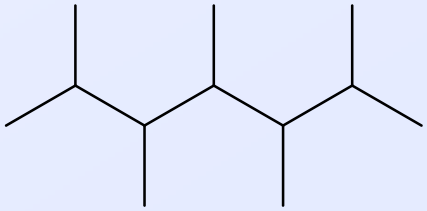




    - Heptamethylnonane
    - Iso-dodecane (2 isomers)



2,2,4,6,6-pentamethylheptane



2,3,4,5,6-pentamethylheptane

  - methyl alkanes

Biodiesel fuels

Recent developments for simulation of kinetics in engines

Ellen Meeks

Session on Contribution of Chemical Kinetics to IC engines
Nara, Japan
29 July 2010

Outline

- **Advanced fuel models and mechanism analysis**
  - Model Fuels Consortium
  - Surrogate-blend approach
  - Automated accurate mechanism reduction
- **Advanced solver approach for incorporating chemical kinetics in CFD**
  - FORTÉ Simulation Package

Reaction Design's core business = kinetics

We are in the business of:

- **Accurate Reacting Flow Simulation**
  - – FORTÉ™ Computational Fluid Dynamics Simulation (*new)*
    - 3-D Turbulent reacting flow for IC engine design
  - – ENERGICO™ Software
    - Emissions and stability prediction for gas turbine engine design
  - – CHEMKIN-PRO® and CHEMKIN-CFD/API™ Software
    - Exclusive worldwide distributor & developer since 1997
    - API provides kinetics solver plug-in for CFD and powertrain simulation
- **Professional Services**
  - – Chemical kinetics and reacting-flow applications
  - – Mechanism development, validation, reduction
  - – Custom software
- **Industry-led Consortia**

toward the development of clean technology

reaction DESIGN

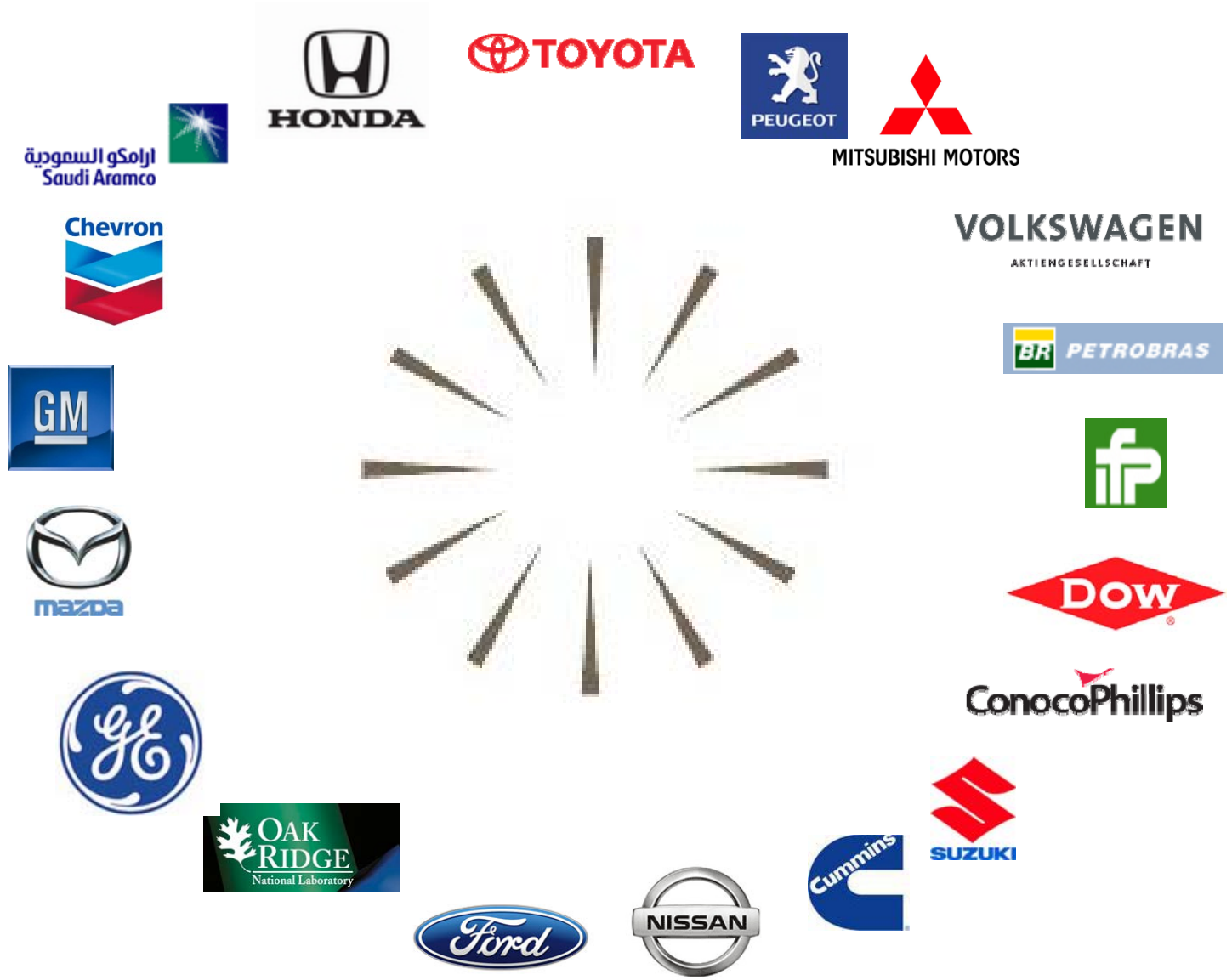
We formed the Model Fuels Consortium to address challenges in engine simulation

- Industry funded and directed
- Built on commercial offerings
- Advised by leading science experts
- Three-year project (Phase 1)
- MFC-II now underway

☞ **Goal is to advance the usability of detailed kinetics in practical engine simulation**

reaction DESIGN

Model Fuel Consortium Members



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MFC Technical Advisory Team

- **Dr. Charles Westbrook – Chief Technical Advisor**
  - A pioneer in combustion modeling while at the Lawrence Livermore National Laboratory
- **Prof. Hiromitsu Ando, Fukui University**
  - Former deputy general manager of engine research at Mitsubishi Motors
- **Prof. Anthony Dean, Colorado School of Mines**
  - Expert kineticist; formerly lead scientist at Exxon
- **Prof. William Green, Massachusetts Inst. of Technology**
  - Expert in numerical methods for model reduction and mechanism generation techniques
- **Prof. Mitsuo Koshi, University of Tokyo**
  - Expert in combustion kinetics and mechanism generation
- **Prof. Ulrich Maas, Universität Karlsruhe**
  - Expert in engine combustion simulation and numerical methods
- **Prof. Rolf Reitz, University of Wisconsin**
  - Expert in engine simulation and engine-design issues
- **Prof. Angela Violi, University of Michigan**
  - Expert in nanoparticle science, fuel-surrogate modeling

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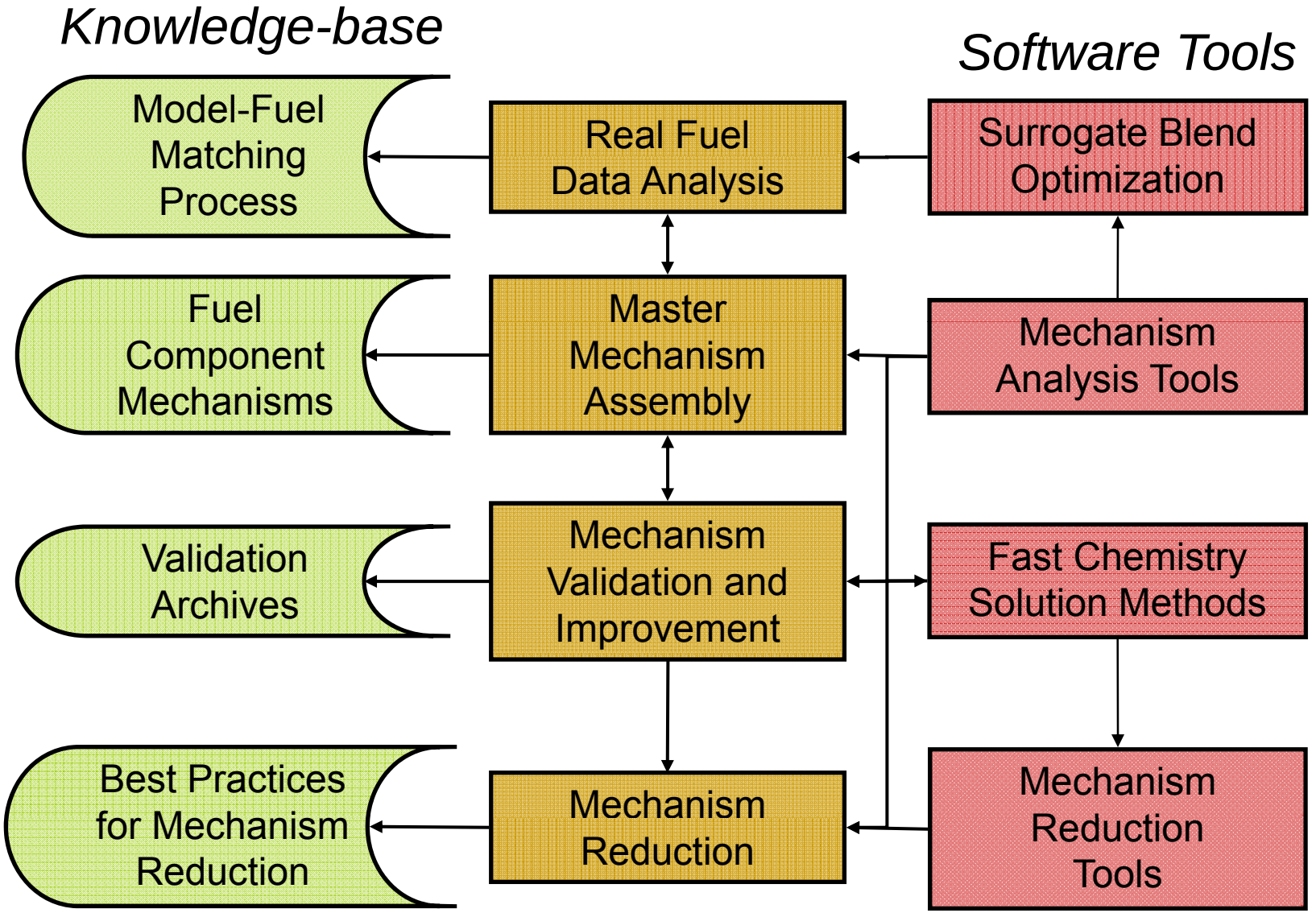
Focus is on building a knowledge-base as well as engineering software tools



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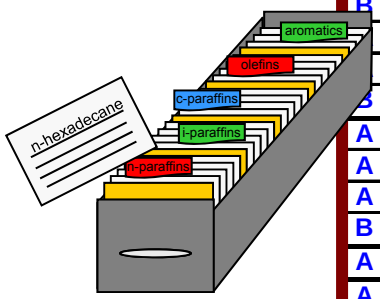
MFC/MFC-II have produced consolidated mechanisms that are internally consistent

Fuel Class	Fuel Component	Year Incorporated	Original Source	Validation Study	Original Rating	Improved	Current Rating
	n-heptane	2006	LLNL/MFC	✓	B	✓	A
n-							A
							A
							A
iso							A
							B
1-ring							B
							B
							A
							A
							A
2-ring							B
							B
cyclo							A
							B
							B
o							A
							B
							B
							A
b							A
							A
							B
fuel							A
Em							A
							D

- **26 component fuels with acceptable (A to B) ratings in "master" surrogates:**
  - n-alkanes: 4
  - iso-alkanes: 2
  - cycloalkanes: 3
  - 1-ring aromatics: 5
  - 2-ring aromatics: 2
  - olefins: 5
  - biofuels: 4
  - additive: 1
- **NO_x emission mechanism improved significantly**
- **Major improvements to core C_0-C_4**



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Mechanism validation and improvement have focused on fundamental experiments

- **Types of data considered:**
  - Shock-tube
  - Rapid Compression Machine
  - Flow Reactors
  - Flames
  - Laboratory engines
- **Over 400 sets of experiments have been modeled to test the mechanisms**
  - CHEMKIN project archives allow continuous testing / improvement
- **Mechanism testing leads to improvements for:**
  - Performance of component-fuel and fuel-blend predictions
  - Mechanism-generation rules
  - Mechanism consistency

The MFC mechanisms allow accurate representation of liquid and gaseous fuels

- **Liquid Fuels**
  - Gasoline
  - Diesel
  - Biodiesel
  - Jet fuel
  - F-T and bio-derived jet
- **Gaseous Fuels**
  - Natural gas
  - GTL
  - Syngas
- **Emissions sub-models for NO_x and soot**

	Relevant to modeling:		
Fuel component	**Gasoline**	**Diesel**	**Jet Fuel**
n-heptane	✓	✓	
n-decane	✓	✓	✓
n-dodecane		✓	✓
n-hexadecane		✓	
i-octane	✓	✓	✓
heptamethylnonane		✓	✓
Toluene	✓	✓	✓
n-propylbenzene	✓	✓	✓
o-xylene	✓	✓	✓
m-xylene	✓	✓	✓
p-xylene	✓	✓	✓
naphthalene		✓	
1-methylnaphthalene	✓	✓	✓
Cyclohexane	✓	✓	✓
Methylcyclohexane	✓	✓	✓
Decalin	✓	✓	✓
1-pentene	✓	✓	
2-pentene	✓	✓	
1-hexene	✓	✓	✓
2-hexene	✓	✓	✓
3-hexene	✓	✓	✓
Ethanol			
DME			
Methylbutanoate			
Methylstearate			
ETBE			
NOx	✓	✓	✓
PAH pathways	✓	✓	✓
Soot	✓	✓	✓

Software analysis tools have also been important outcomes from the MFC

Reaction Workbench

- **Surrogate Blend Optimizer**
- **Mechanism Reduction with user control of error**
- **Mechanism Merge, Extract, Compare Utilities**

CHEMKIN-PRO

- **Reaction Path Analyzer**
- **New reactor models**
  - Multi-zone HCCI engine model
  - Laminar flame extinction model
- **Solver improvements**
  - Fast and robust flame simulations
  - Dramatic speed up of closed homogeneous reactors

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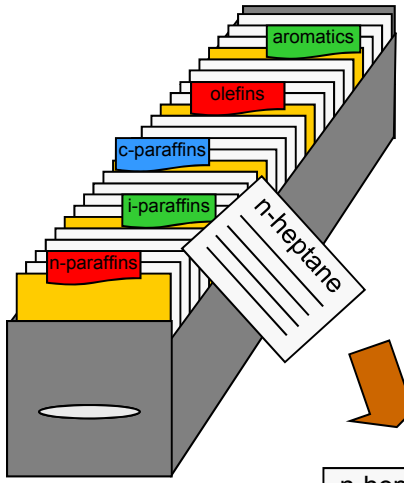
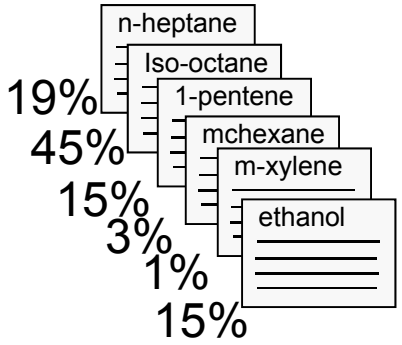
The Surrogate Blend Optimizer facilitates matching model-fuel to real-fuel properties





Set Target Characteristics
- Class composition
- Heating value
- Octane / Cetane #
- H/C ratio, O content
- Boiling points
- Sooting threshold index

Other physical properties

Fuel properties to match

Choose Fuel Palette
Select Components to Include in the Surrogate

Match Properties
- Optimize Composition

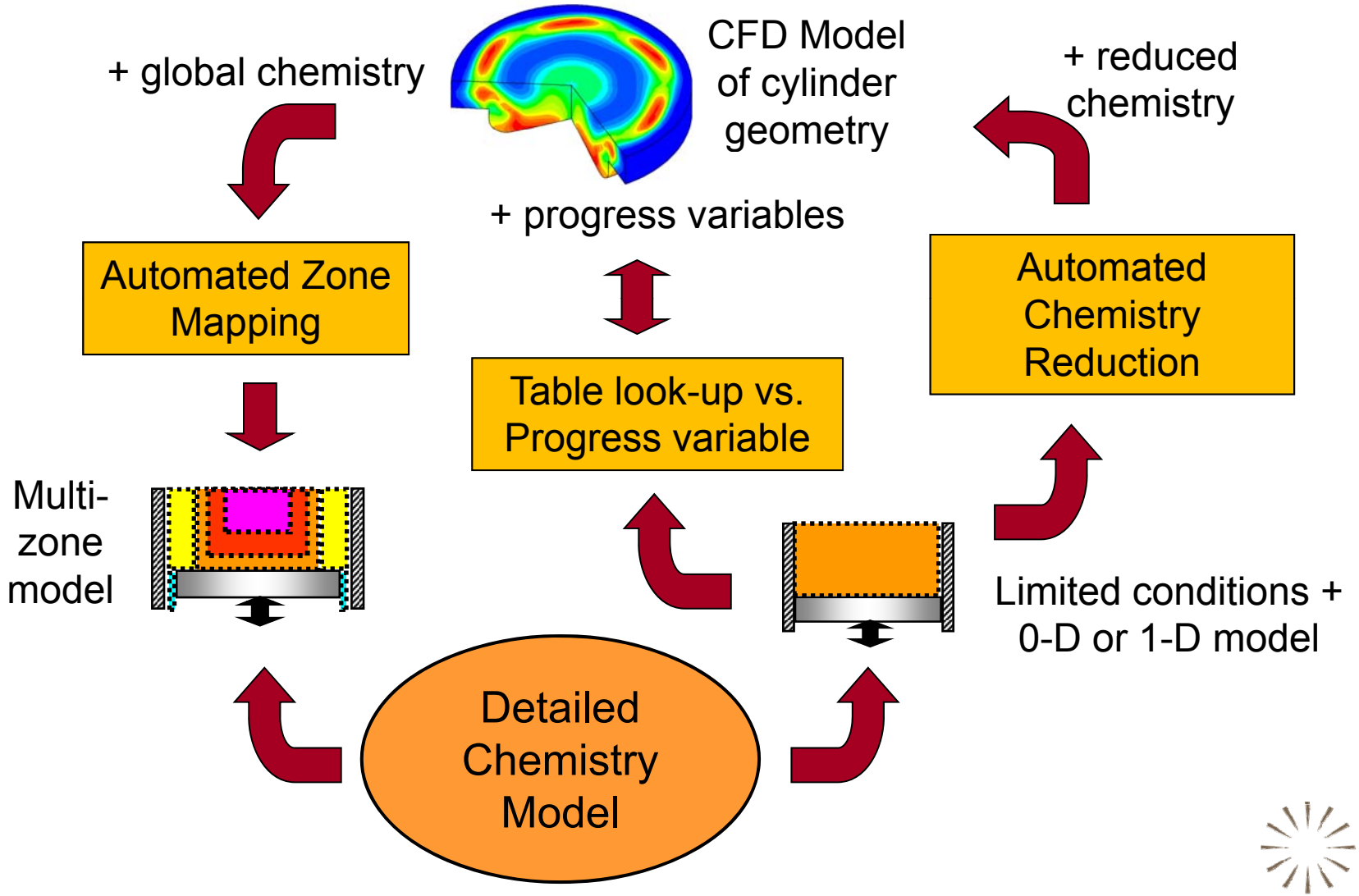
Surrogate Fuel Composition

Chemical Model for Simulation

Mechanism Reduction, as necessary

reaction DESIGN

There are several ways to use accurate kinetics data in engine simulation

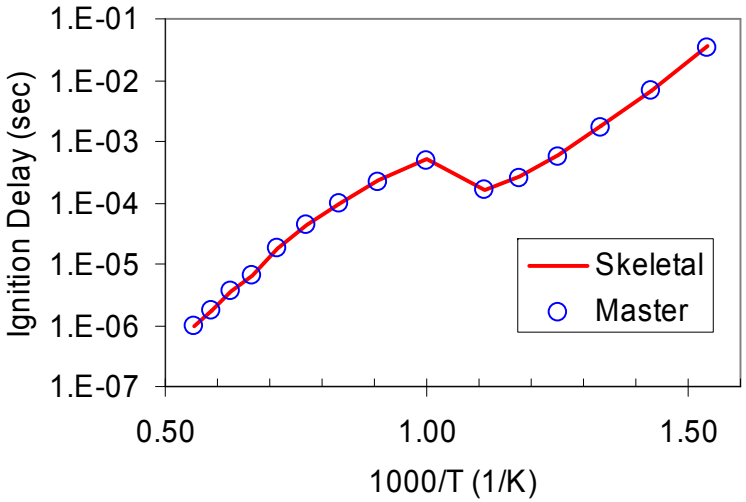


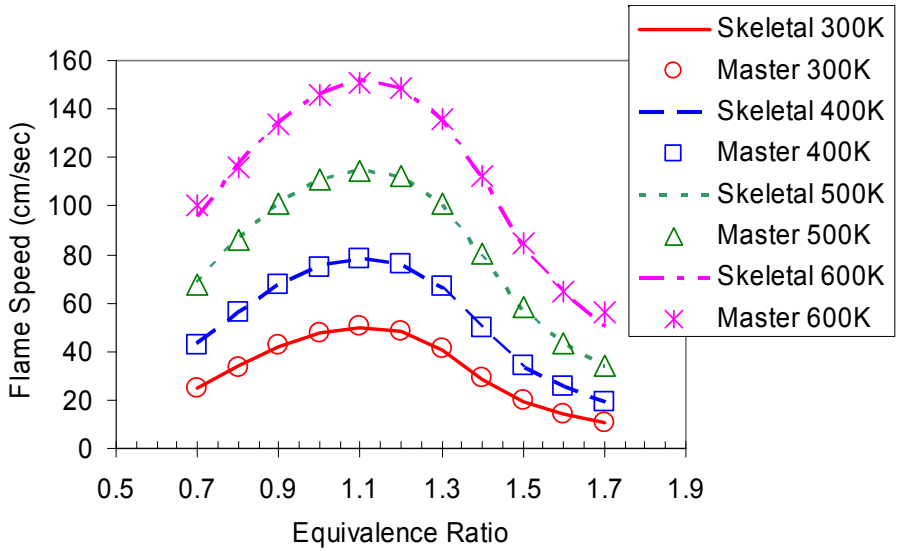
reaction DESIGN

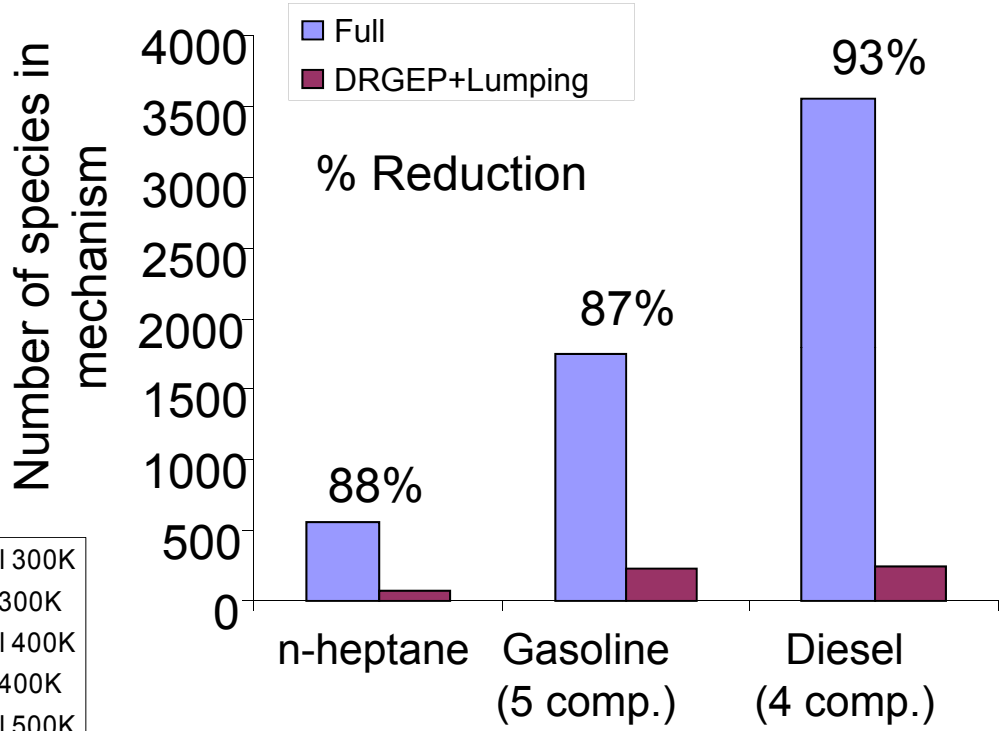
Advanced mechanism-reduction techniques keep accuracy with more reduction

- **Skeletal methods that track error and sensitivity, based on Directed Relation Graph**
  - Fine tune the reduction process to achieve more effective reduction
- **User control of error in simulation target**
  - E.g., ignition time, flame-speed, emissions
  - Iterative reduction until acceptable error is reached
- **Automated lumping of selected species**
  - Use SMILES identifiers to select and process species and reaction data during lumping

Multi-component surrogate models can be accurately reduced to ~100s of species







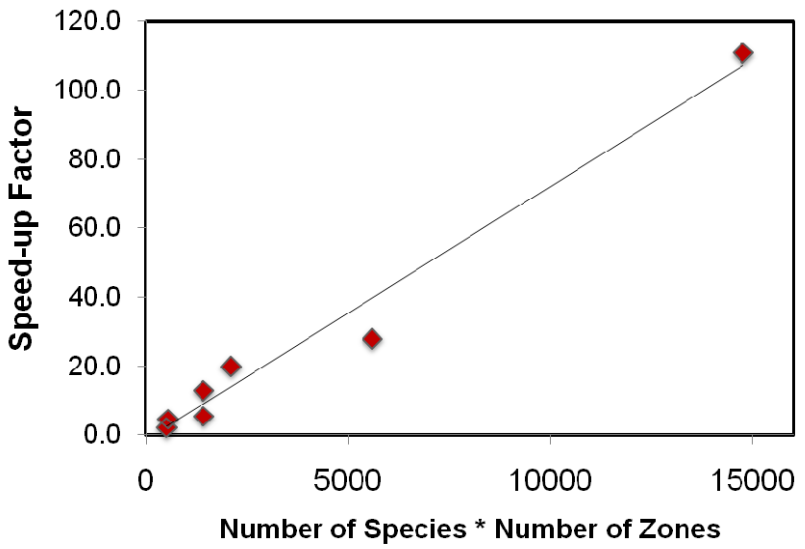
reaction DESIGN

Another way we allow more chemistry accuracy is through improved solvers

- Solver improvements take advantage of sparsity in large chemistry systems

Problem Description	# Species	# Zones	CPU time (h:m:s)		Speed -up
			Before	After	
Closed system – MFC gasoline	1440	1	0:11:36	0:02:03	**5.7**
Closed system – n-hexadecane	2116	1	0:20:15	0:01:00	**20.3**
Multi-zone Engine – GRI-mech	53	10	0:00:36	0:00:16	**2.3**
Multi-zone Engine – n-heptane	561	10	1:26:01	0:03:03	**28.2**
Multi-zone Engine – 5-component	1477	10	56:14:17	0:30:28	**110.8**

- Hours => a few minutes
- n^2 scaling => ~n



Benchmarks from a 64-bit Linux Blade server (Dual Core Xeon Processor, 4MB Cache, 2.0GHz, 1333MHZ FSB forPowerEdge 1955, 16GB RAM)

reaction DESIGN

There are 3 main goals for MFC-II

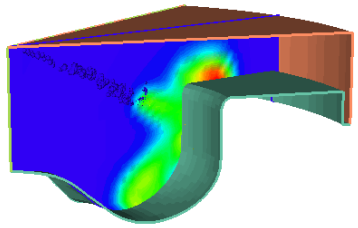
- **Continue building and validating the Mechanism Database, with focus on Alternative Fuels**
  - Future fuels, blends and additives; aromatics formation
  - Continuous improvement
  - Database management
- **Develop and validate predictive soot models**
  - Soot formation, oxidation and particle size prediction
  - Effects of fuel changes and fuel blends
  - Obtain fundamental experimental data to support
- **Advance the ability to use detailed kinetics in CFD**
  - Support use of detailed kinetics in engineering simulation
  - Focus on new technology that bridges the divide between speed and accuracy

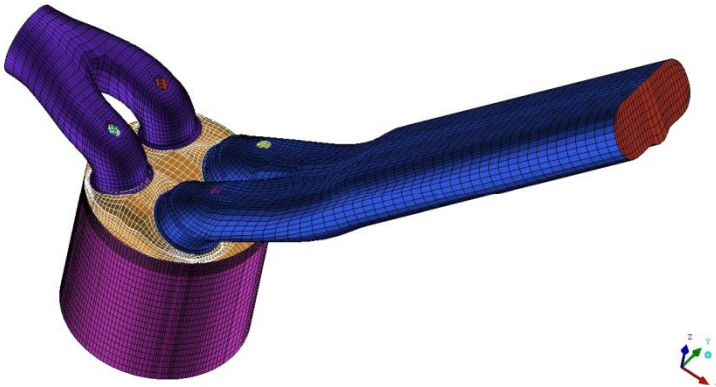
Almost every engine company we talk to is "re-evaluating" their combustion CFD tools

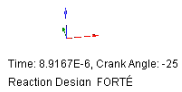
- **Not satisfied with current offerings:**
  - Can't handle the chemistry needed for fuel effects / emissions
    - Solutions take too long
    - Fuel representations are too simple (e.g., reduced n-heptane)
    - Simulations are not robust (often fail to converge)
    - Emissions models (esp. soot) give wrong trends/results
  - Too much fitting/calibration needed to match experimental data; not sufficiently predictive
  - Don't get support they need from CFD companies

reaction
DESIGN

Introducing a New 3-D Engine Simulation Capability - FORTÉ







We developed FORTÉ to address engine-simulation with detailed chemistry

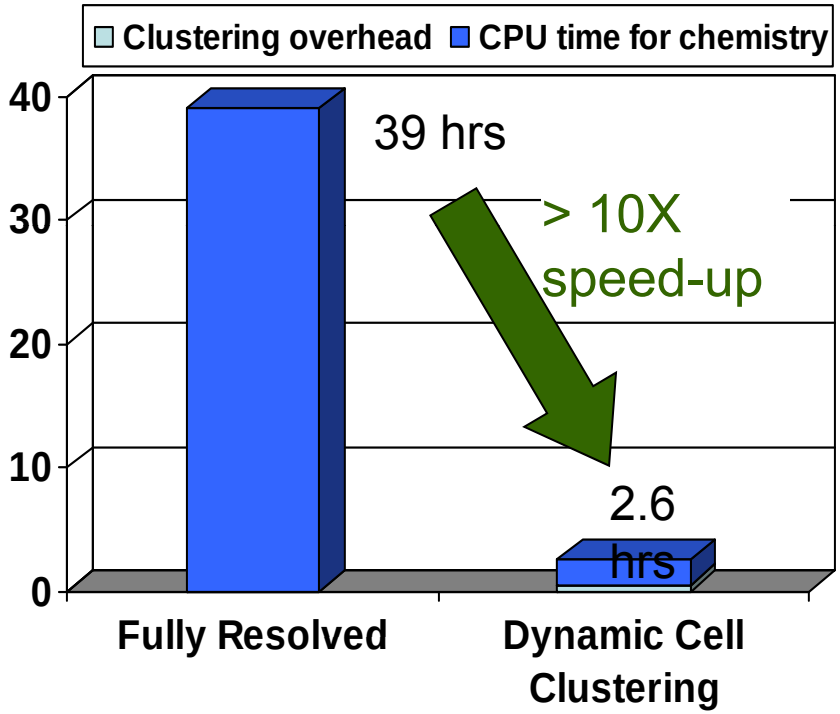
- **Realistic representation of auto fuels (MFC)**
  - Accurate mechanisms for surrogate-blend components, for engine operation
    - Relevant range of pressure, temperature, equivalence ratio
  - Accurate emissions models
    - NO_x, soot (MFC-II)
- **Consistency between spray and chemical model**
  - Accurate surrogate blend
    - Chemical and physical properties matched
    - Multicomponent spray-vaporization model
- **Automated and accurate mechanism reduction**
  - Advanced skeletalization and species-lumping methods

RD's chemistry solvers represent a big advance over other commercial tools

- **Very efficient full-accuracy solution as base**
  - Sparse-matrix solution makes no approximation
- **Dynamic Adaptive Chemistry option**
  - On-the-fly reduction of kinetics to that needed at local time, local space in the engine cycle
  - Minimal user input required
- **Dynamic Cell Clustering chemistry option**
  - Collects kinetically similar cells to reduce repetition
  - Minimal user input required
- **Parallel computing**
  - For distributed-node and multi-CPU configurations

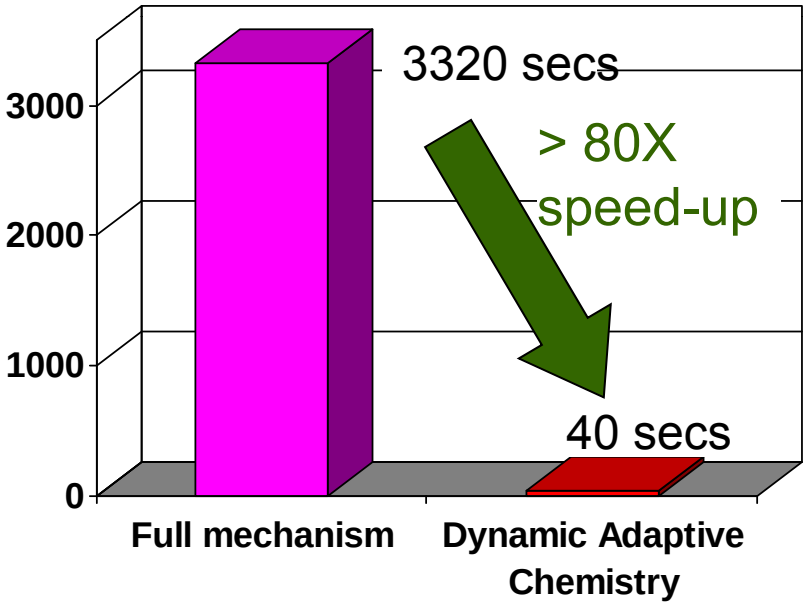
Unprecedented speed means more detailed mechanisms can be used with less time

- **Dynamic cell clustering can reduce time by > 10X**



Example is for 36-species n-heptane mechanism, for a diesel sector mesh

- Dynamic adaptive chemistry can *further* reduce time by > 80X



Example is for 310-species n-hexadecane mechanism, for a single-cell test HCCI test case

reaction DESIGN

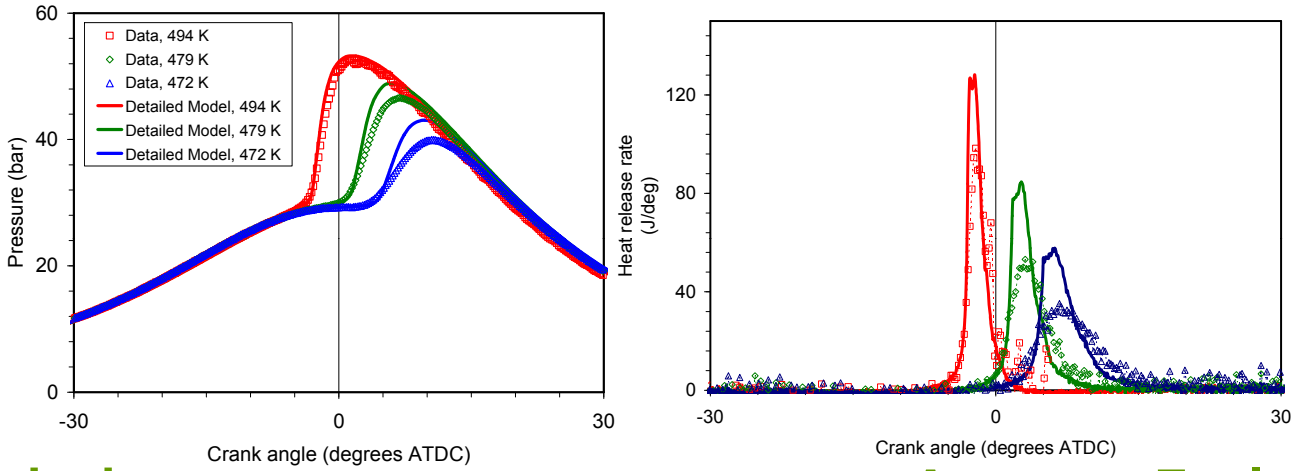
Most chemistry models in use by industry today are not sufficiently predictive

- **They are used in combination with extensive calibration of spray, ignition timing, emissions models, etc. to match data**
  - OK for conventional Diesel engine design
- **High-efficiency, clean-combustion strategies hinge much more on the kinetics themselves**
  - E.g., premixed charge, low-temperature conditions
- **The best test of the kinetics model is in simulations of HCCI or PCCI engine data**
  - Less opportunity to compensate via the spray model

A fully detailed kinetics mechanism, however, provides accurate combustion predictions

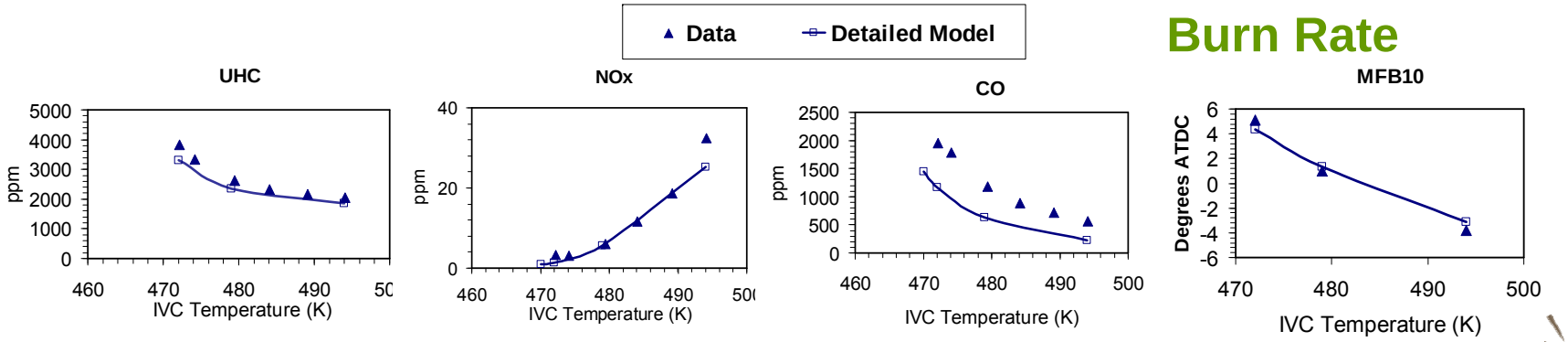
- **HCCI engine w/ detailed PRF/ethanol mechanism**
  - 428 species; skeletal version of a well validated MFC mechanism

Accurate Ignition Timing



Accurate Emissions

Accurate Fuel Burn Rate



Puduppakkam, et al., SAE Paper Series 2010-01-0362
Data is from B. Bunting, ORNL

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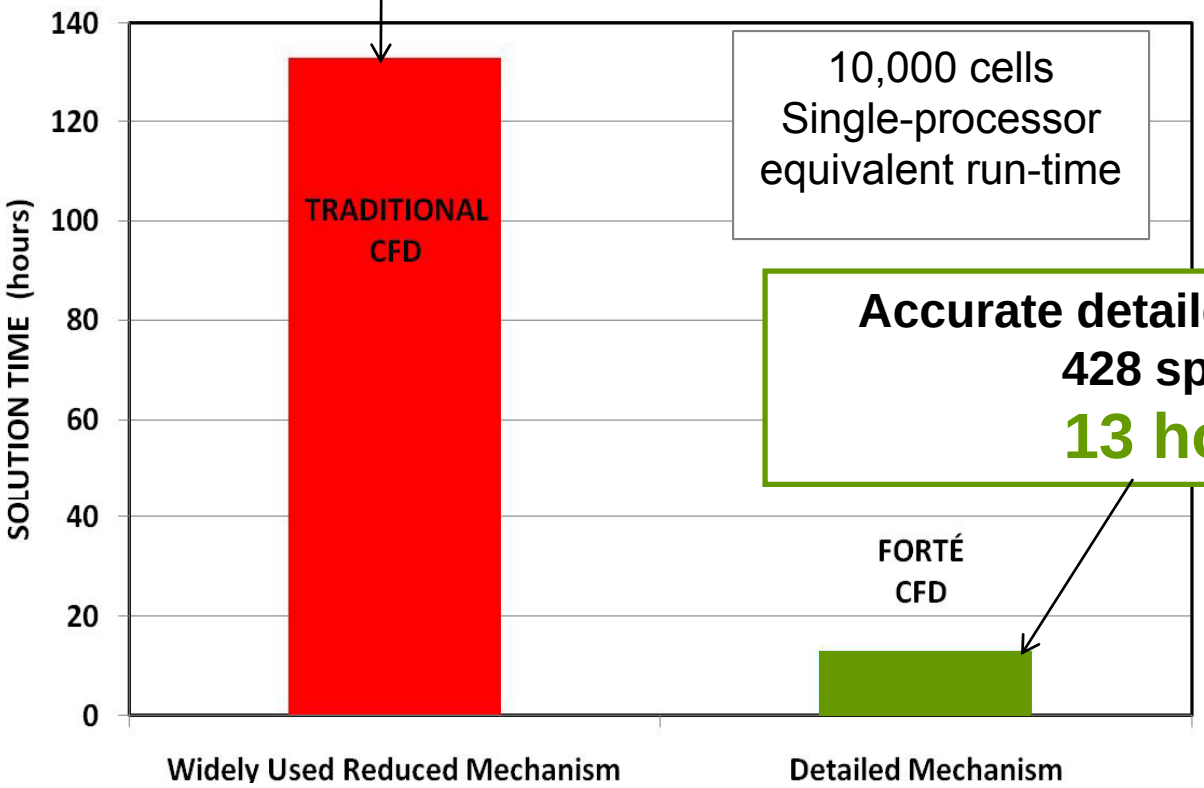
FORTÉ Benchmark for HCCI conditions

Widely used reduced mechanism
~100 species
without advanced solver
133 hours

HCCI Engine running
PRF+Ethanol Fuel Blend



10,000 cells
Single-processor
equivalent run-time

Accurate detailed mechanism
428 species
13 hours

reaction DESIGN

We partnered with WERC to bring in advanced spray models that further improve accuracy

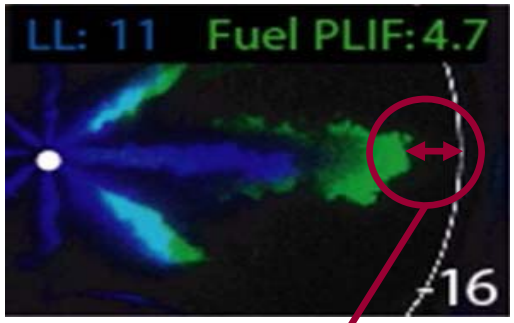
- **"Grid-independent" spray representation**
  - State-of-the-art representation of spray physics:
    - Nozzle flow model
    - Droplet break-up model
    - Gas-jet model (reduces grid dependency)
    - Droplet collision model
  - Allows more accurate spray model without the need to drastically increase mesh refinement
  - Less calibration necessary due to improved accuracy for a given grid
- **Significant reduction in time-step dependence as well**

A model of an optical engine at Sandia shows the capability for spray + kinetics

- **Model of the Cummins optical engine at Sandia National Labs**
  - Detailed fuel surrogate used to model diesel
    - 51% n-tetradecane
    - 33.5% n-decane
    - 15.5% 1-methyl naphthalene
  - 45 degree sector mesh
  - 437 species detailed mechanism used
  - Multi-component fuel vaporization
  - Low temperature combustion
  - Early injection

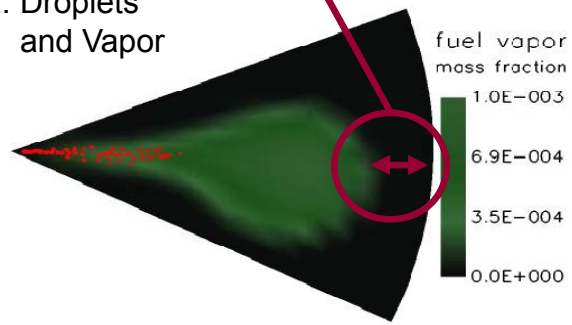
FORTÉ spray model results show accurate ignition and spray penetration

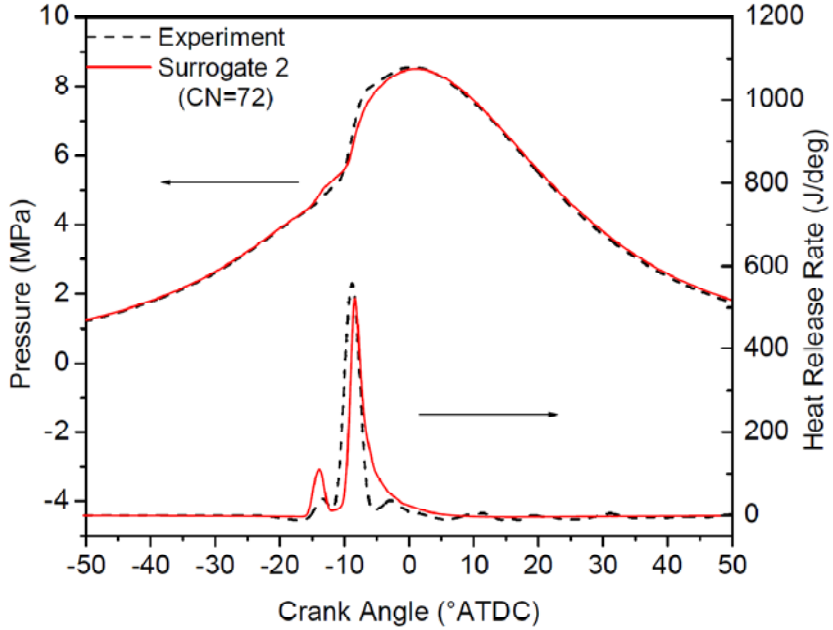
Data: Spray and Fuel PLIF



Good spray penetration

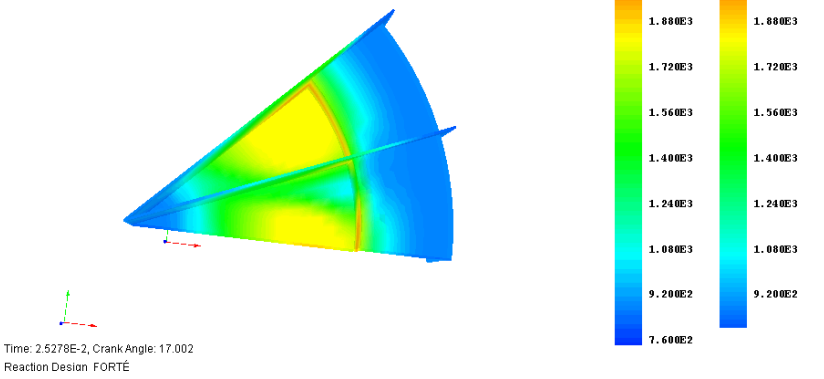
FORTÉ: Droplets and Vapor





Liang, et al., SAE Paper Series, 2010-01-0178

Data are from Cummins engine studied at Sandia National Labs by S. Singh, M.P.B. Musculus, R.D. Reitz, SAE Paper 2006-01-0055.



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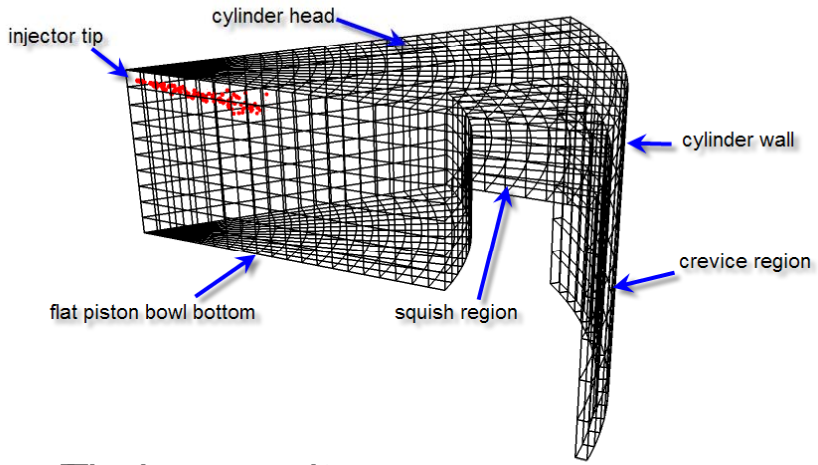
Realistic fuel models can be used with < 1-day turn-around

- **Example: Diesel engine-sector simulation**



Model Fuel Matches:

- C/H Ratio
- Lower Heating Value of Fuel
- T50 boiling point value
- Consists of:
  - 51% n-tetradecane
  - 33.5% n-decane
  - 15.5% 1-methyl naphthalene

Timing results:

Total CPU time (4 cpus)	Chemistry Time per cpu	Total time (1-cpu equivalent)
12 h , 28 min	8 h, 30 min	44 hours, 44 min

Multicomponent fuel model is used with detailed kinetics in ~ 12 hours with 4 CPUs

Liang, et al., SAE Paper Series, 2010-01-0178

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Fast solution in FORTÉ enables real-fuel chemistry for clean engine design

- **Realistic modeling of fuel effects is now a key issue in engine design**
- **Accurate, fast chemistry simulation is required for**
  - Predictive ignition calculations
  - Predictive emissions calculations
- **FORTÉ brings together fast chemistry solvers with the most accurate, efficient spray models**
  - Multiple chemistry solver speed-up options
  - Spray model's grid-independent results allow coarser meshs
- **FORTÉ is customized for engine designers**
  - Guided set-up, run and visualization

reaction DESIGN