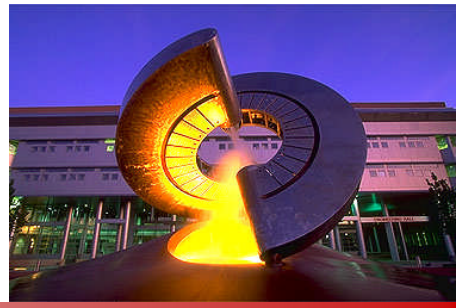
Reciprocating Internal Combustion Engines

Prof. Rolf D. Reitz,
Engine Research Center,
University of Wisconsin-Madison

2012 Princeton-CEFRC
Summer Program on Combustion
Course Length: 9 hrs

(Wed., Thur., Fri., June 27-29)

Hour 3



Short course outine:

Engine fundamentals and performance metrics, computer modeling supported by in-depth understanding of fundamental engine processes and detailed experiments in engine design optimization.

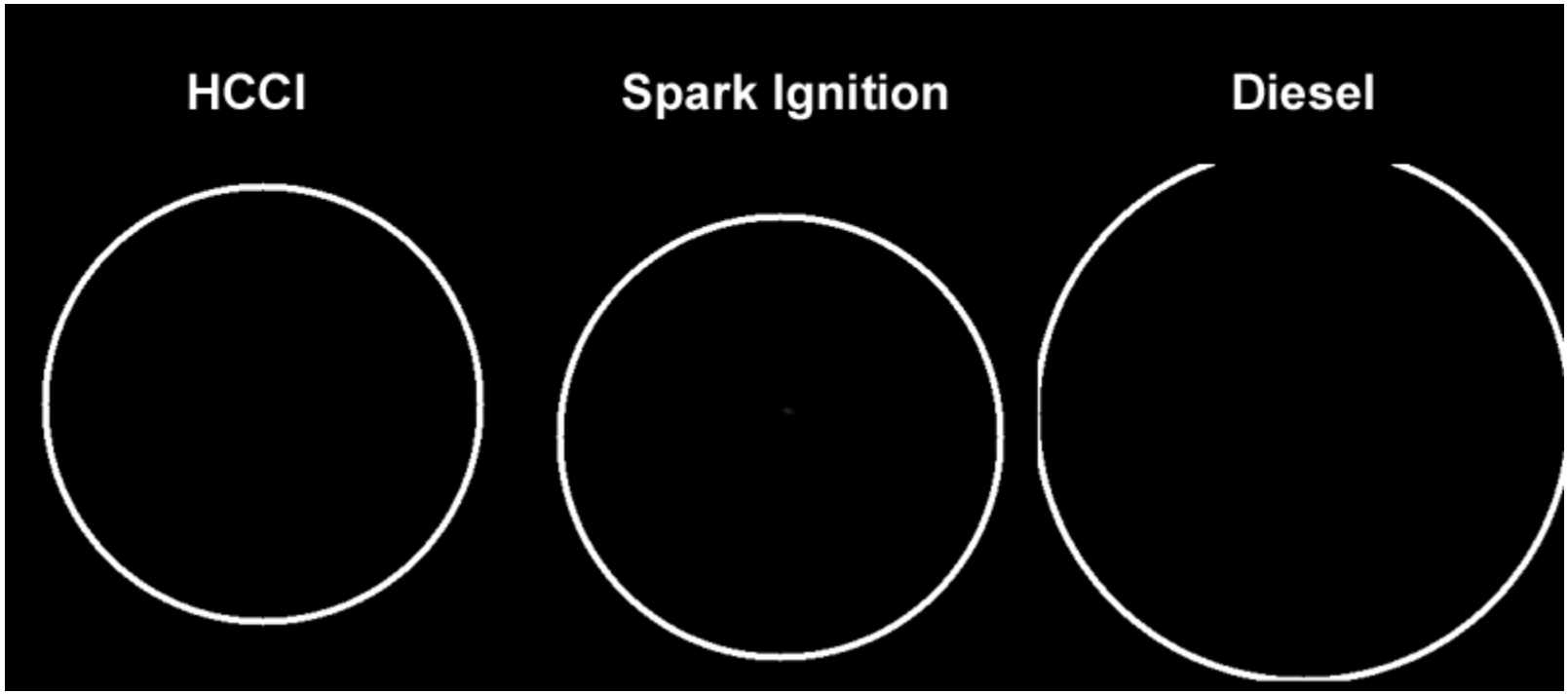
Day 1 (Engine fundamentals)
Hour 1: IC Engine Review, 0, 1 and 3-D modeling
Hour 2: Turbochargers, Engine Performance Metrics
Hour 3: Chemical Kinetics, HCCI & SI Combustion

Day 2 (Spray combustion modeling)
Hour 4: Atomization, Drop Breakup/Coalescence
Hour 5: Drop Drag/Wall Impinge/Vaporization
Hour 6: Heat transfer, NOx and Soot Emissions

Day 3 (Applications)
Hour 7: Diesel combustion and SI knock modeling
Hour 8: Optimization and Low Temperature Combustion
Hour 9: Automotive applications and the Future

Modes of Engine Combustion

http://www.erc.wisc.edu/combustion.php

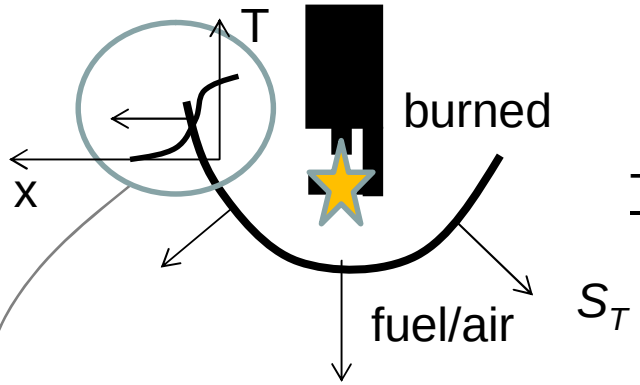


HCCI uses a hybrid combustion strategy. Premixed fuel and air is inducted, but instead of igniting with a spark as in a SI engine, the high temperature from compression causes the mixture to spontaneously react, like in a diesel engine. Ignition occurs at slightly different times at different locations in the chamber.

One feature of HCCI combustion is how quickly the fuel is consumed.

Basic Combustion Concepts – Spark Ignition (SI)

How can SI engines operate with engine speeds from 100 to 20,000 rev/min?



Turbulence!

- Kinetic energy, $k \sim V_{piston}^2$
- Integral length scale $l_I \sim L_{piston}$
- Kinetic energy dissipation rate, $\varepsilon \sim V_{piston}^3 / L_{piston}$
- Diffusivity, $D \sim k^2/\varepsilon \sim V_{piston} L_{piston}$

Because turbulent flame speed, S_T, scales with rpm!

Characteristic Time Combustion (CTC) model — Reitz & Bracco, 1983; Abraham, 1985

Species conversion rate (Y_i, species mass fraction, * local equilibrium solution)

$$\frac{dY_i}{dt} = -\frac{Y_i - Y_i^*}{\tau_c} \quad ; \quad \tau_c \sim k/\varepsilon \sim L_{piston} / V_{piston}$$

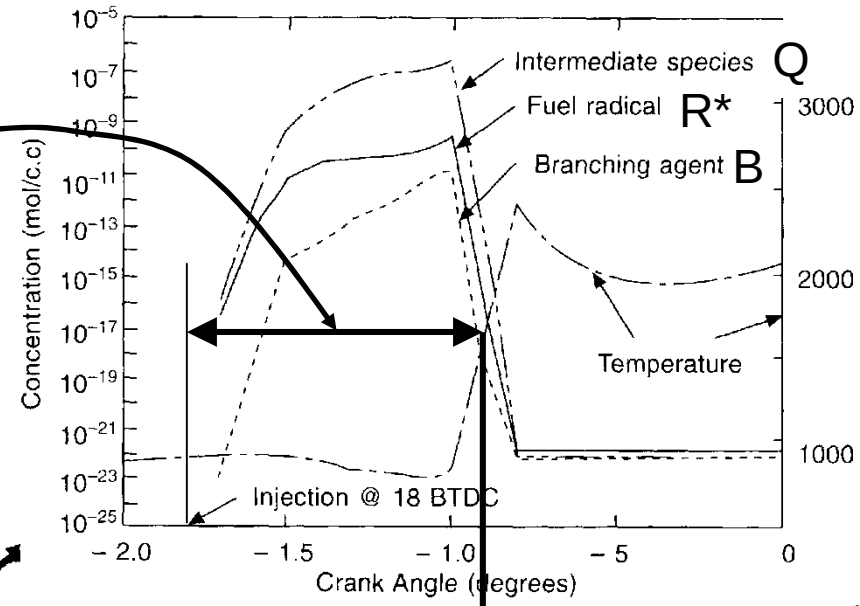
Mallard-Le Chatelier propagating wave speed:

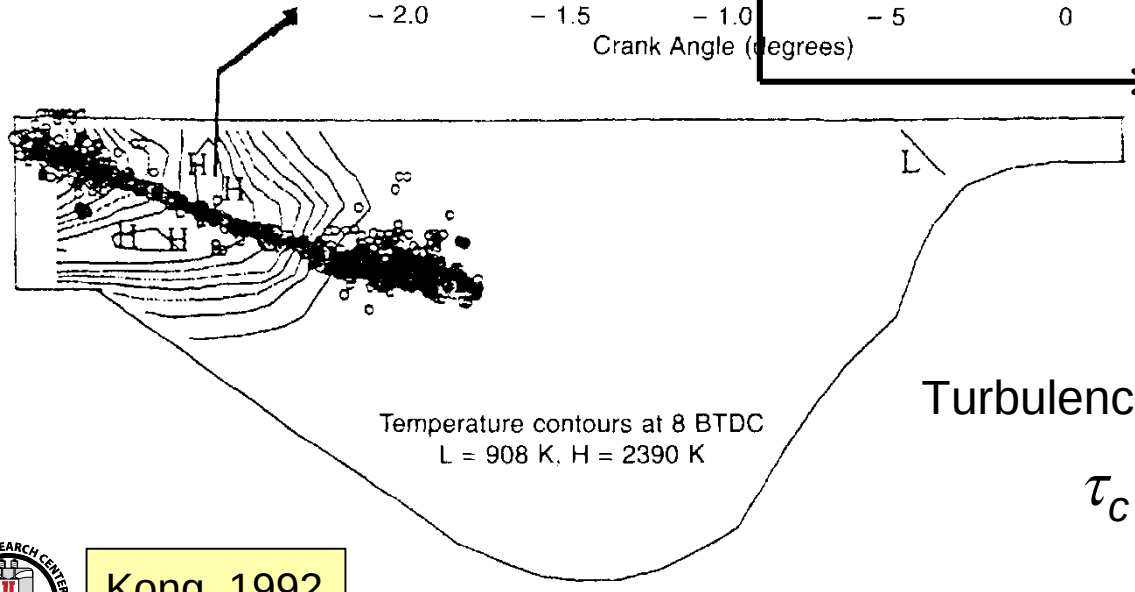
$$S_T = \sqrt{D \frac{dY_i}{dt}} \sim V_{piston}$$

Glassman, 1996

Basic Combustion Concepts – Diesel (CI)

Ignition Delay





Kong, 1992

Halstead, 1977

Shell Ignition Model

$RH + O_2$	→	2R*	
R*	→	R* + P + Heat	
R*	→	R* + B	
R*	→	R* + Q	← Af04
R* + Q	→	R* + B	
B	→	2R*	
R*	→	termination	
2R*	→	termination	

Switch to Characteristic Time Combustion model

$$\frac{dY_i}{dt} = -\frac{Y_i - Y_i^*}{\tau_c}$$

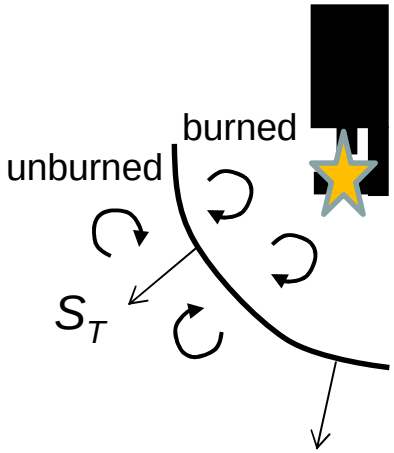
Turbulence generated by fuel injection

$$\tau_c \sim k/\varepsilon \sim L_{nozzle} / V_{nozzle}$$

Turbulent Mixing

Spark-ignition

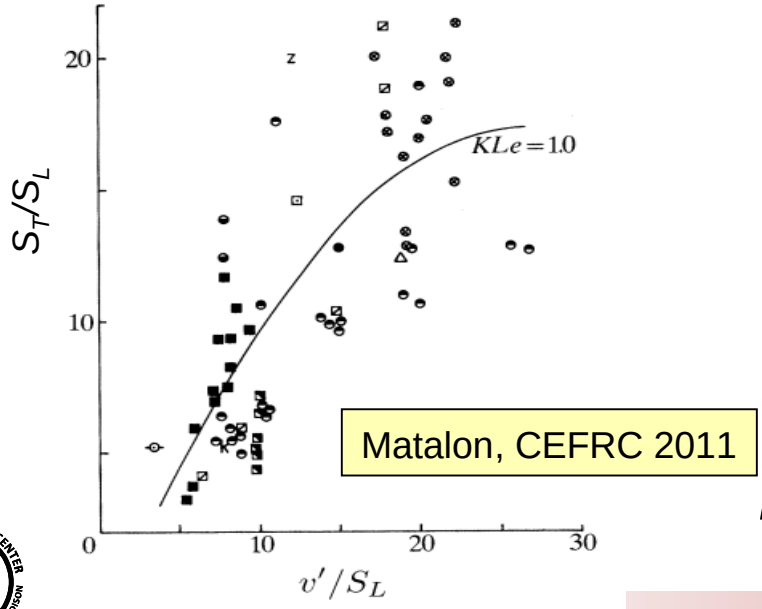
Hot products with
Cold reactants



$\tau \sim k/\varepsilon$

$\sim L_{piston} / V_{piston}$

High turbulence
- faster combustion



Matalon, CEFRC 2011

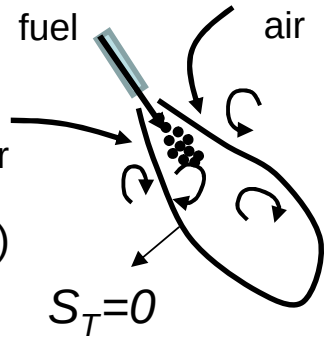
Diesel

Injected fuel with
entrained air

$\tau \sim k/\varepsilon$

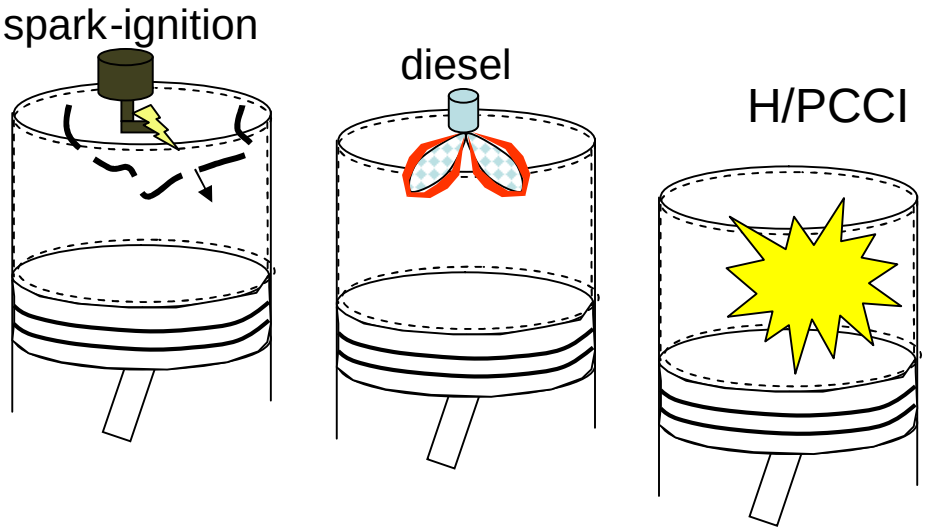
$\sim L_{nozzle} / V_{nozzle}$

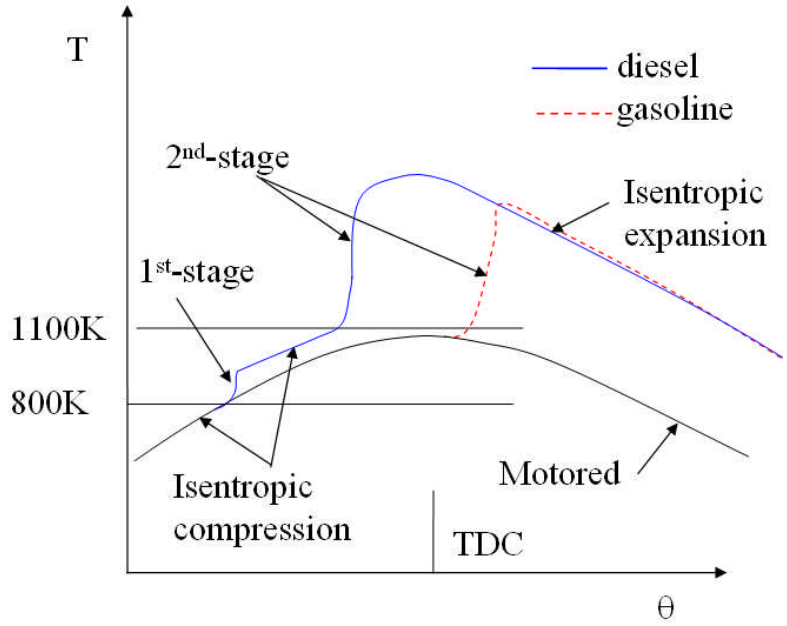
Delayed ignition (PCCI)
- better mixing



Summary of combustion regimes

- Gasoline engine spark-ignition with flame propagation:
  High turbulence for high flame speed → heat losses. Issues: NOx and UHC/CO, knock (CR, fuels), throttling losses → low thermal efficiency TE ~25%
- Diesel engine with spray (diffusion) combustion:
  Rich mixtures (soot) & high temperatures (NOx) → higher TE ~45%
- H/Premixed Charge Compression Ignition – LTC, chemistry controlled:
  Sensitive to fuel, poor combustion/load control, low NOx-soot → TE ~50%



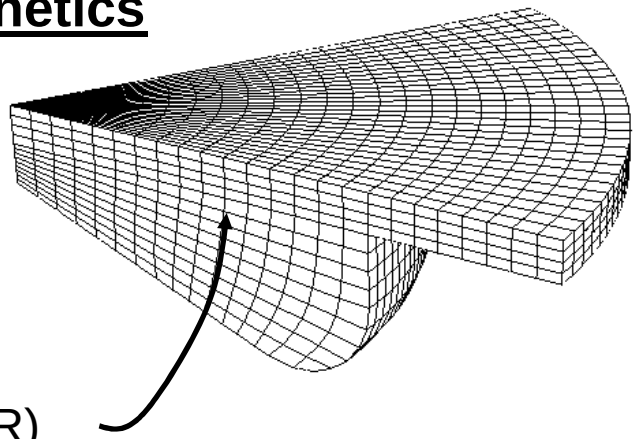


Premixed Volumetric Combustion & Chemical Kinetics

Species and energy conservation equations

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i u) = \nabla \cdot [\rho D \nabla (\frac{\rho_i}{\rho})] + \dot{\rho}_i^c + \dot{\rho}_i^s$$

$$\frac{\partial (\rho I)}{\partial t} + \nabla \bullet (\rho \mathbf{u} I) = -p \nabla \bullet \mathbf{u} - \nabla \bullet \mathbf{J} + \rho \varepsilon + \dot{Q}^c + \dot{Q}^s + \dot{Q}^r$$



Constant volume combustion – Well-Stirred-Reactor (WSR)

$$\frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} \left(\nu''_{k,i} - \nu'_{k,i}\right) q_k(\mathbf{Y}, T), \qquad i = 1, \cdots, n_s$$

$$\sum_{i=1}^{n_s} \nu'_{k,i} M_i \rightleftharpoons \sum_{i=1}^{n_s} \nu''_{k,i} M_i, \qquad k = 1, \cdots, n_r$$

$$q_k(\mathbf{Y}, T) = \kappa_{f,k} \prod_{i=1}^{n_s} \left(\frac{\rho Y_i}{W_i}\right)^{\nu'_{k,i}} - \kappa_{b,k} \prod_{i=1}^{n_s} \left(\frac{\rho Y_i}{W_i}\right)^{\nu''_{k,i}}$$

$$\kappa_{f,k}(T) = A_k T^{b_k} \exp\left(-\frac{E_k}{RT}\right) \; ; \qquad \kappa_{b,k}(T) = \kappa_{f,k}(T) / Kc_{eq,k}(T)$$

$$Kc_{eq,k}(T) = \exp\left(-\Delta g_k^0\right) \left(\frac{p_{atm}}{RT}\right)^{\sum_{i=1}^{ns} \left(\nu''_{k,i} - \nu'_{k,i}\right)}$$

$$\frac{dT}{dt}(\mathbf{Y}, T) = -\frac{1}{\bar{c}_v(\mathbf{Y}, T)} \sum_{i=1}^{n_s} \left(\frac{U_i(T)}{W_i} \frac{dY_i}{dt}(\mathbf{Y}, T)\right)$$

Williams, 1988

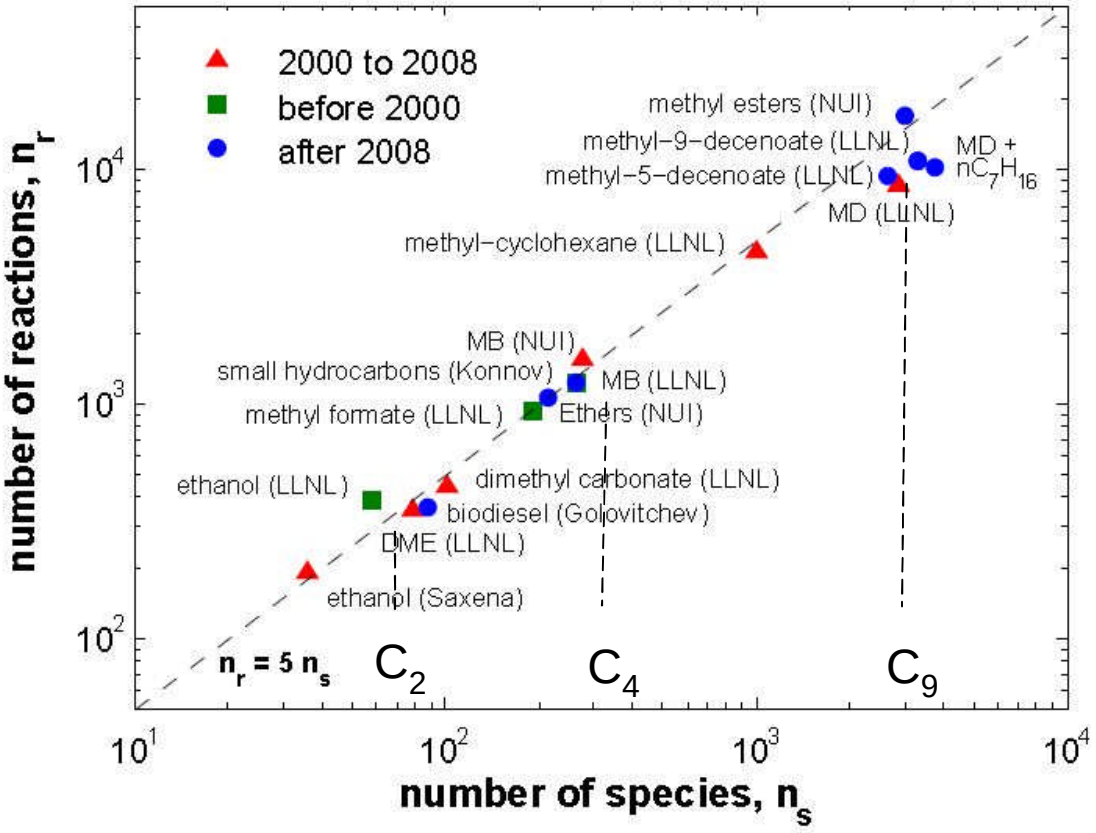
I	specific internal energy
M_i	chemical label
n_r	reactions
n_s	species
$\nu'_{k,i}\, \nu''_{k,i}$	reactant/product stoichiometric coefficients
Y_i	mass fraction
W_i	molecular weight
U_i	species energy

$$U_i = R_{mol} \left[(a_i - 1) T + \frac{b_i}{2} T^2 + \frac{c_i}{3} T^3 + \frac{d_i}{4} T^4 + \frac{e_i}{5} T^5 + f_i\right]$$

Chemical Kinetic Mechanisms for Engine Simulations

Requirements for mechanisms for practical engine simulations:

- Size can not be too large due to CPU time limitation ~ 100 species
- Capable of predicting auto-ignition delay time accurately
- Contain proper reactions for pollutant formation precursors



Biodiesel surrogates

- Significant mechanism reduction is required.

Soy biodiesel - Methyl:

- palmitate (C16:0)
- stearate (C18:0)
- oleate (C18:1)
- linoleate (C18:2)
- linolenate (C18:3)

Hydrocarbon kinetics - NTC

Warnatz, 2006

Second Stage Ignition

$H_2O_2 = OH + OH$

RH

O_2

R → olefin + R

O_2

RO_2

QOOH → olefin + HO_2

QOOH → cyclic ether + OH

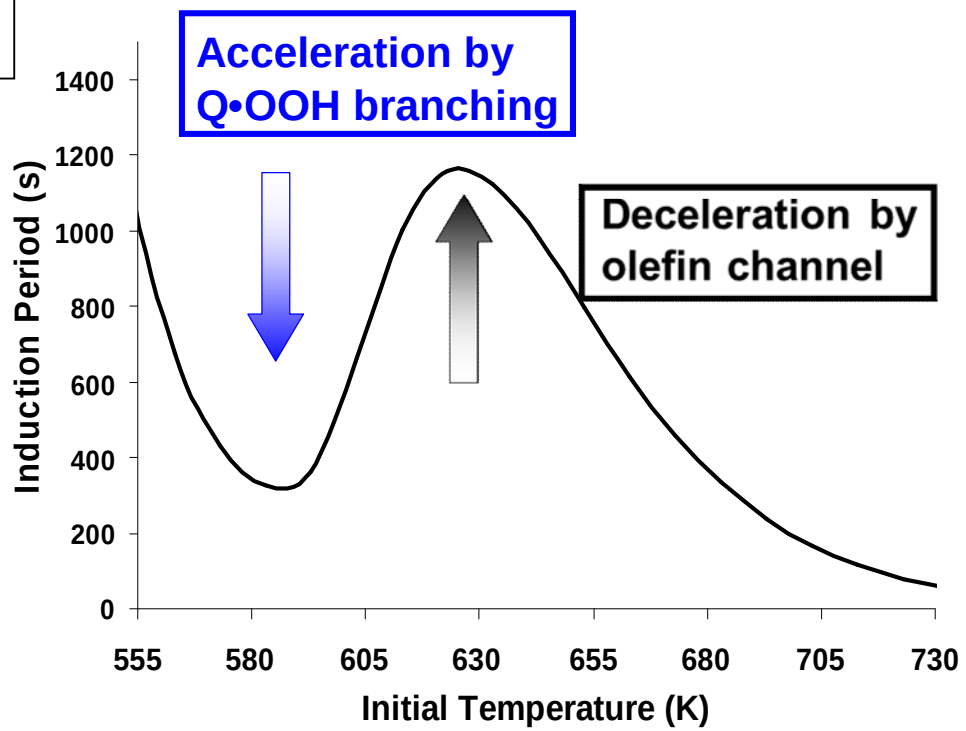
O_2

O_2QOOH → keto-hydroperoxide + OH

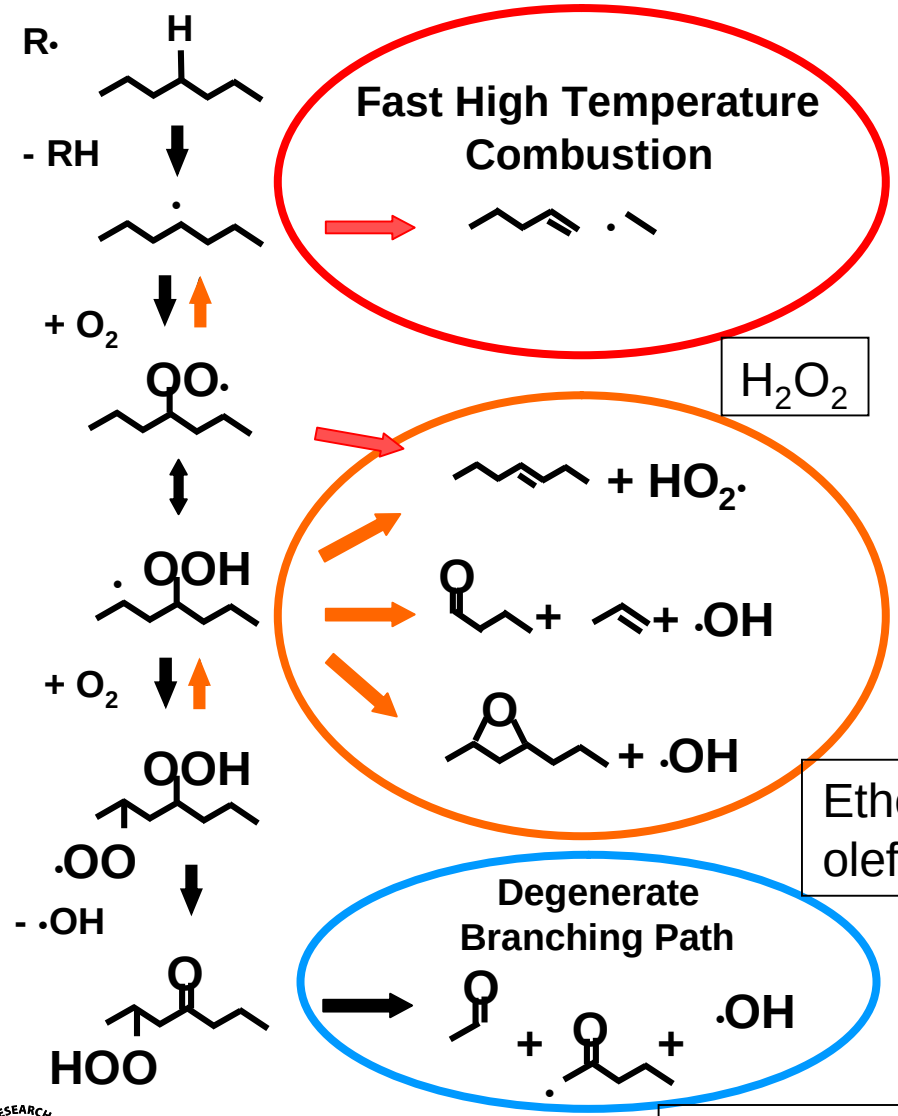
keto-hydroperoxide → (low T branching)

First Stage Ignition

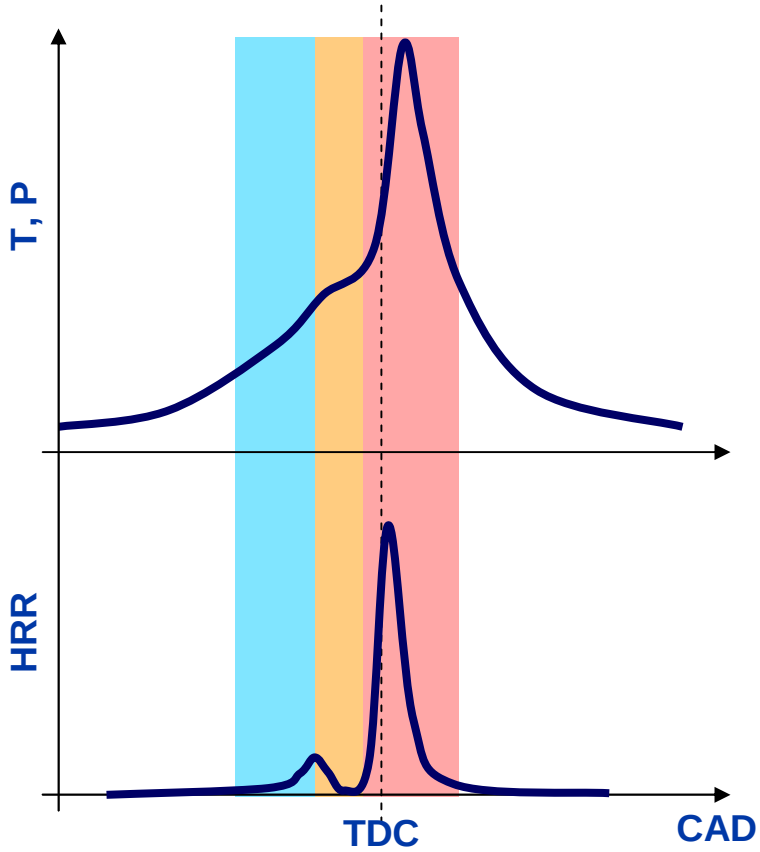
Isomerization steps



HCCI combustion kinetics

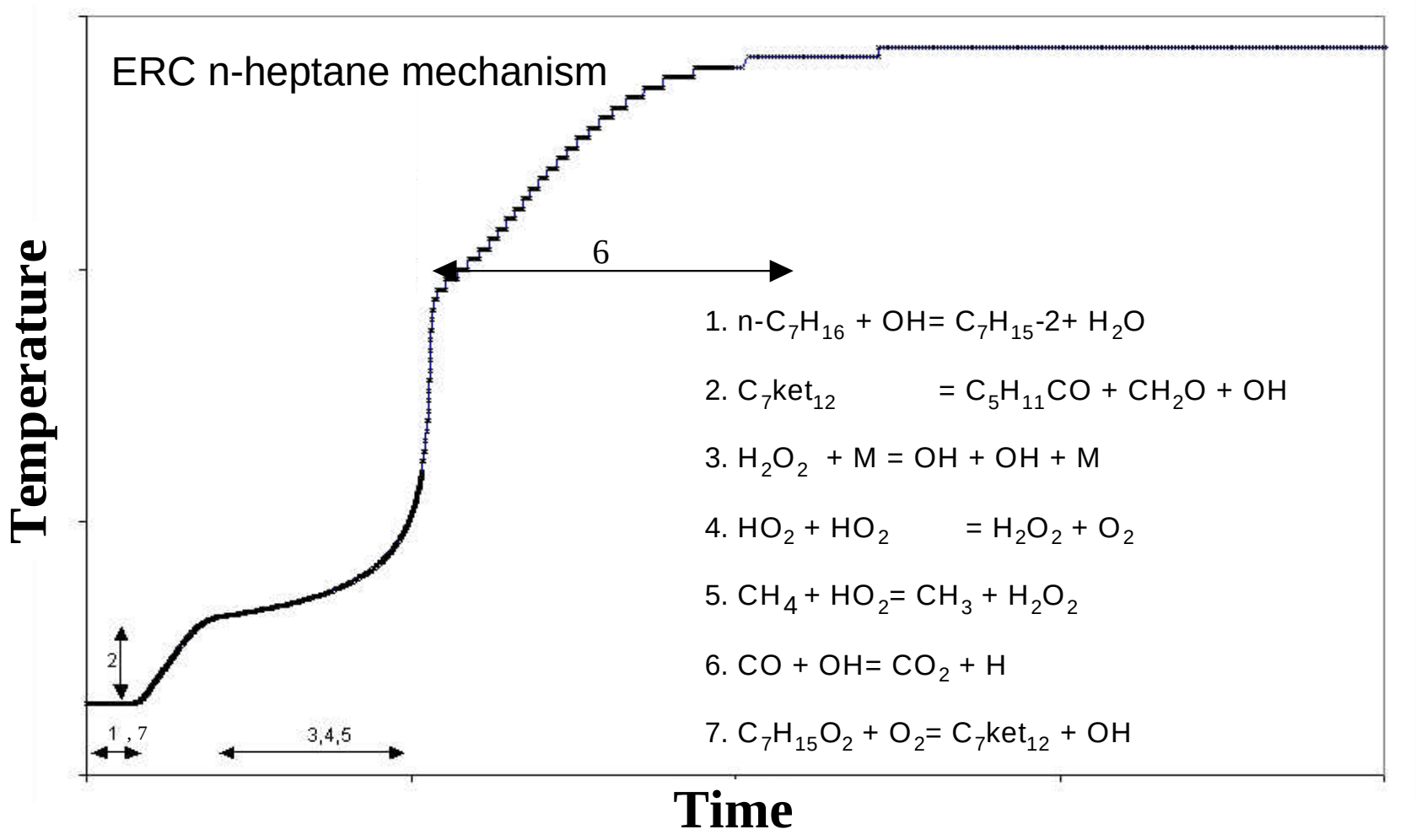


Typical HCCI Combustion Temperature and Heat Release Rate profiles



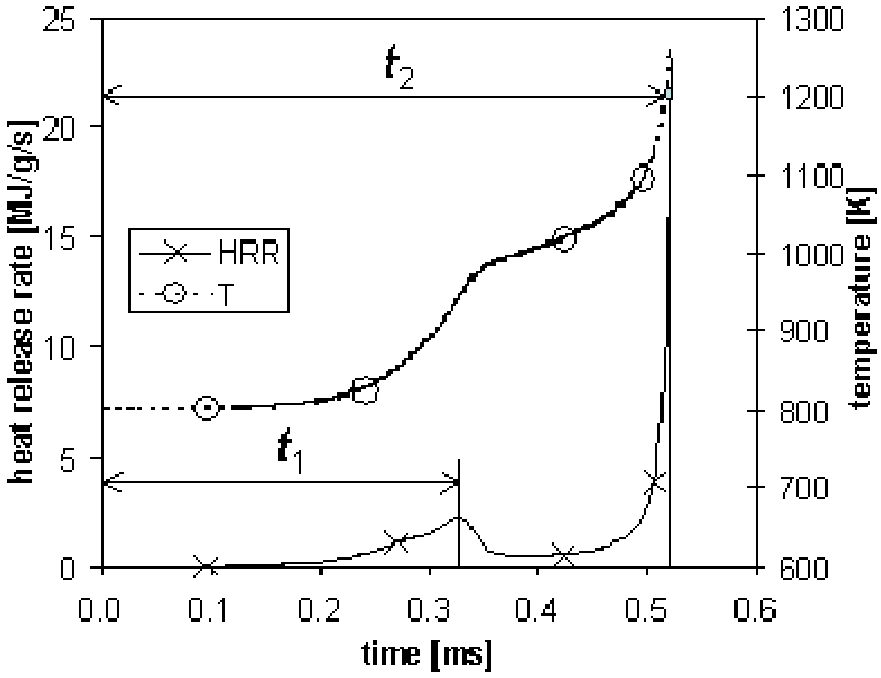
Mehl, 2009

Mechanism reduction – identify key reaction steps



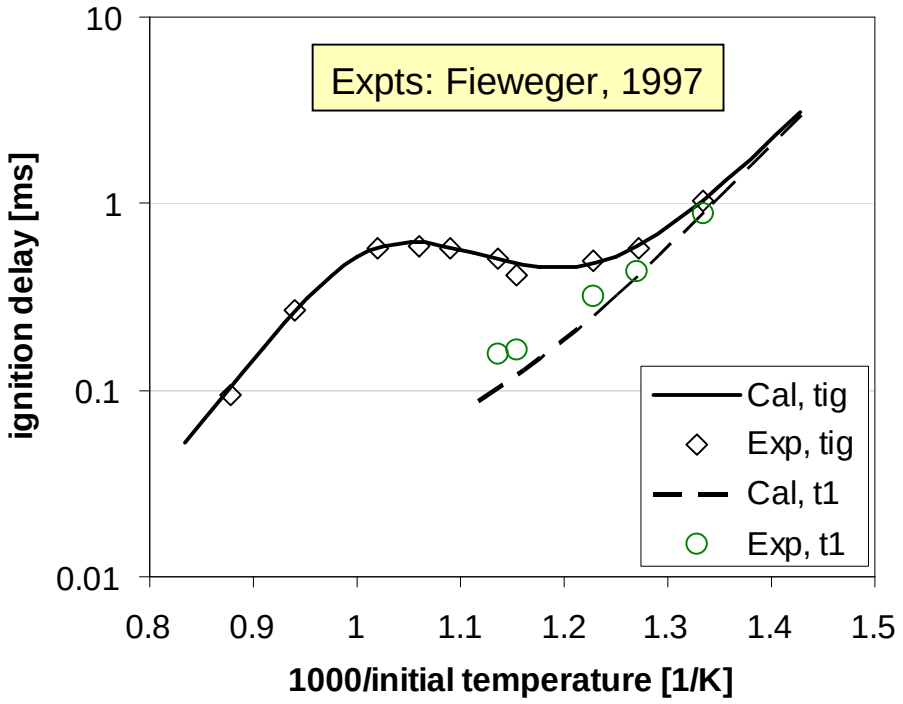
Patel, SAE 2004-01-0558

Reduced mechanisms - match shock tube and RCM data



Predicted ignition delay times validated against shock tube tests (data from Fieweger)
ϕ=1.0 and P=40 bar n-heptane/air

First stage (t1), main ignition (t2=tig) delay



Ra and Reitz, 2008

Mechanism reduction methodology

Reduction of reaction pathways and species number
- combination of chemical lumping, graphical reaction flow analysis and elimination methods

Reaction rate optimization
- ignition delay curve sensitivity analysis

Pre-exponential: $A = k \times A_{base}$

Ignition delay sensitivity coefficient

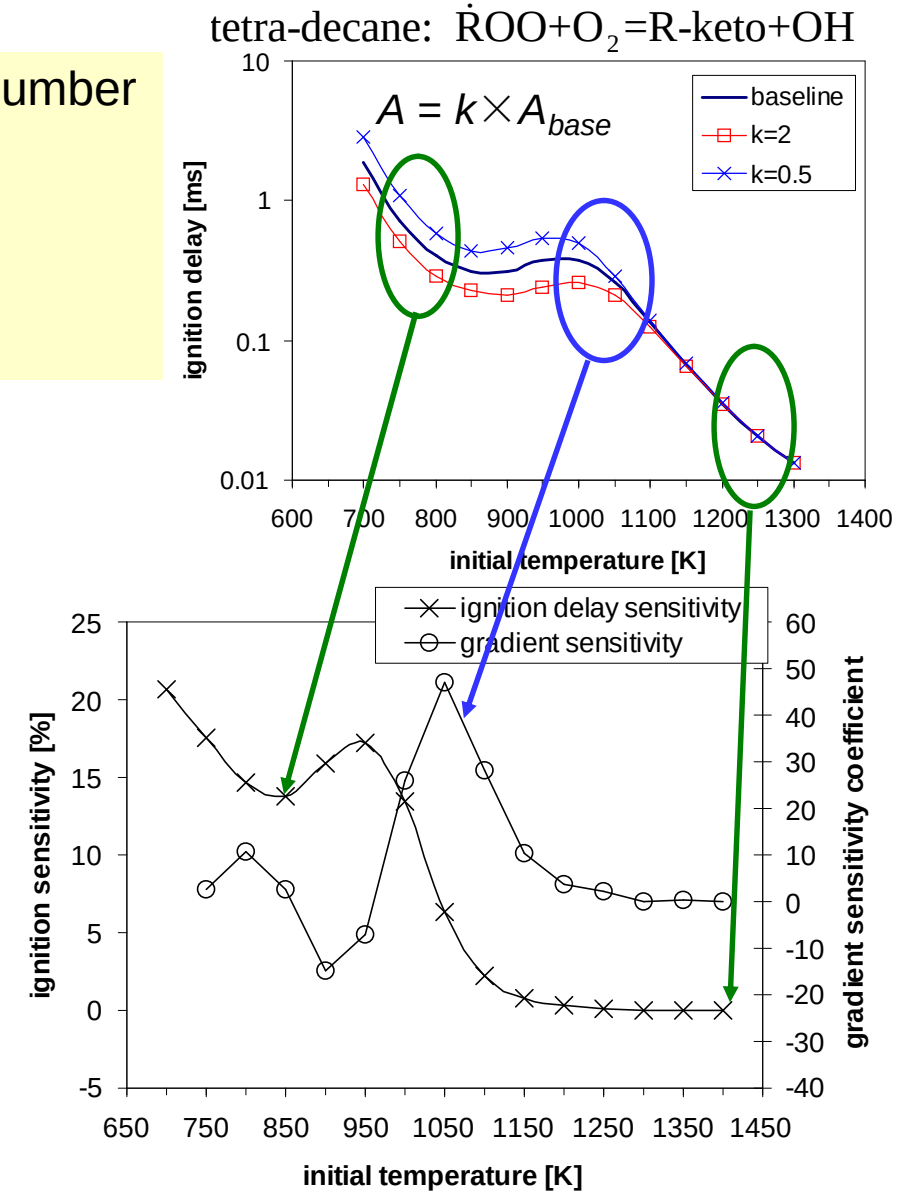
$$S_{ig}(T) = 100 \times \frac{(\log_{10} t_{k_1} - \log_{10} t_{k_2})}{\log_{10} t_{base} \log_{10}(k_1/k_2)}$$

Ignition delay gradient sensitivity coefficient

$$S_{gr}(T) = \frac{\frac{d \log_{10} t_{k_1}}{dT} - \frac{d \log_{10} t_{k_2}}{dT}}{\log_{10}(k_1/k_2)} \times 100$$

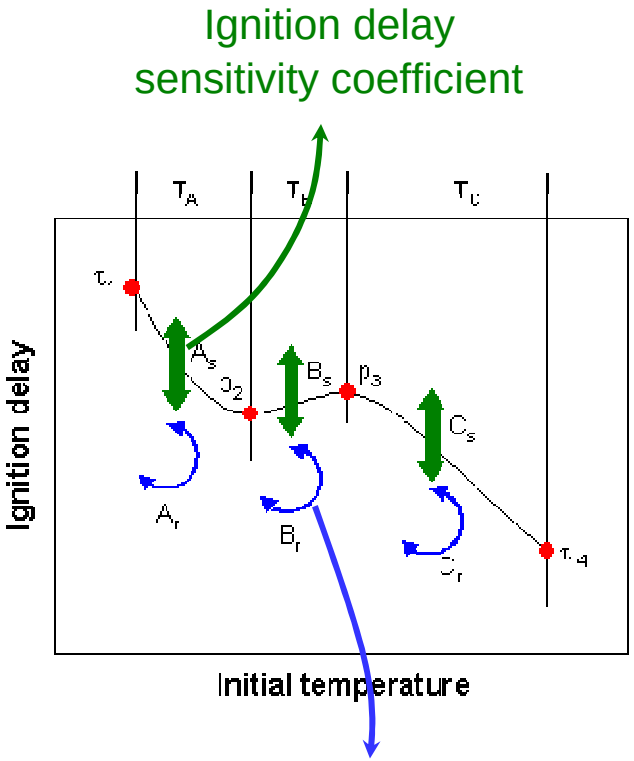
Positive S_{gr}: counter-clockwise rotation
Negative S_{gr}: clockwise rotation

Ra and Reitz, 2011



Mechanism reduction – group reaction classes

No	Reaction	A_s	B_s	C_s	A_r	B_r	C_r	effect
I	$RH + H = \dot{R} + H_2O$							
II	$RH + OH = \dot{R} + H_2O$	●↓		●↑		●C		τ_1, p_2, p_3, τ_4
III	$RH + HO_2 = \dot{R} + H_2O_2$	○↓	○↓	○↓				τ_1, P_2, P_3, τ_4
IV	$RH + O_2 = \dot{R} + HO_2$		○↑	○↓		●		P_2, P_3
V	$\dot{R} + O_2 = R\dot{O}O$							
VI-a	$R\dot{O}O = \dot{Q}OOH$	●↓	●↓			○C		τ_1, P_2
VI-b	$\dot{Q}OOH + O_2 = \dot{O}OQOOH$	○↓	●↓					P_2, P_3
VI-c	$\dot{O}OQOOH$ = R-keto + OH	○↓	●↓					P_2, P_3
VII	R-keto = CH_2O + R'CO + OH	●↓			○C			τ_1
VIII	R'CO = X_1 + X_2 + CO							
IX	$\dot{R} = S_1 + S_2 + S_3$		●↑				○	P_2, P_3, τ_4



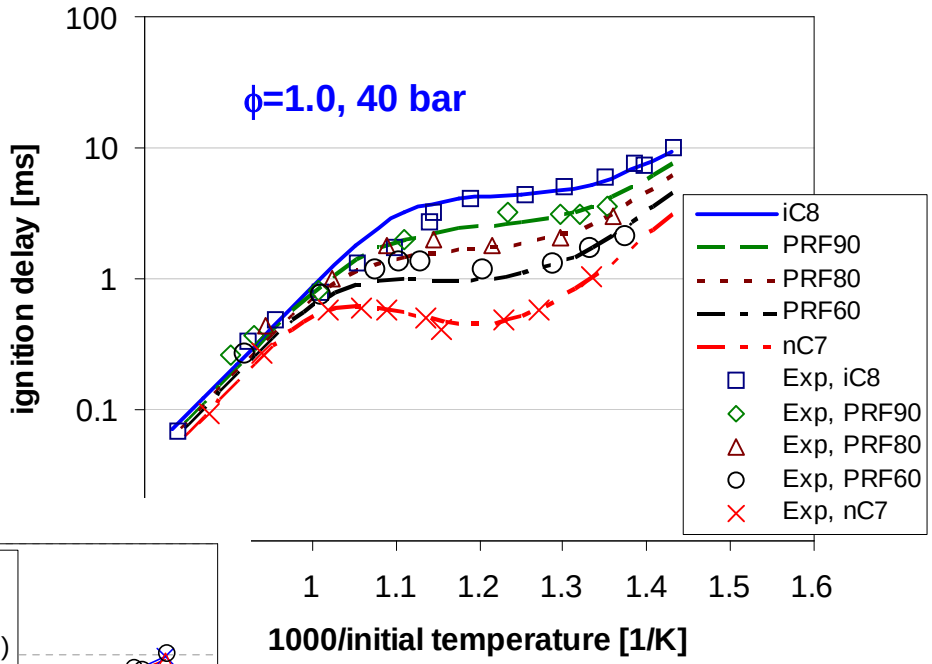
Sensitivity of ignition delay curves of n-heptane oxidation
- solid circle, open circle and blank entry denote dominant, mild and not significant influence, respectively.
- *C* indicates counter-clockwise rotation.
- Circle only indicates clockwise rotation.

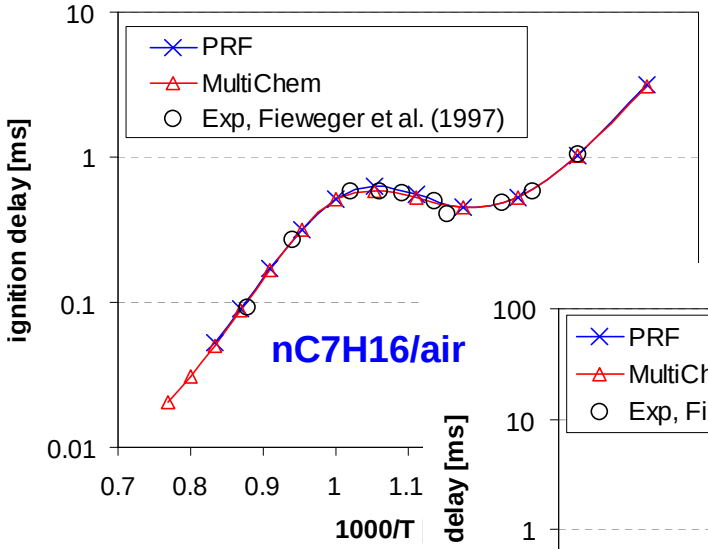
Ra and Reitz, 2011

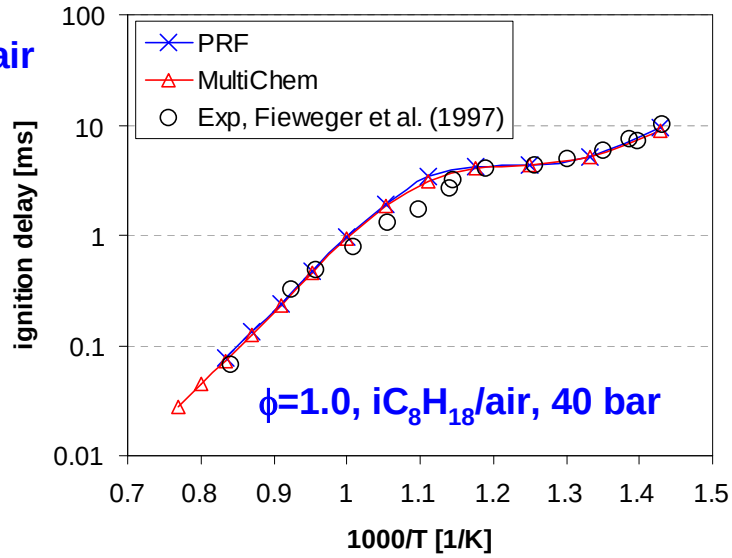
ERC-MultiChem: PRF

41 species, 158 reactions ➔ base mechanism

Source mechanisms: LLNL n-heptane (560 species; 2,539 reactions), isooctane (857 species; 3,606 reactions), ERC n-heptane (29 species; 52 reactions)

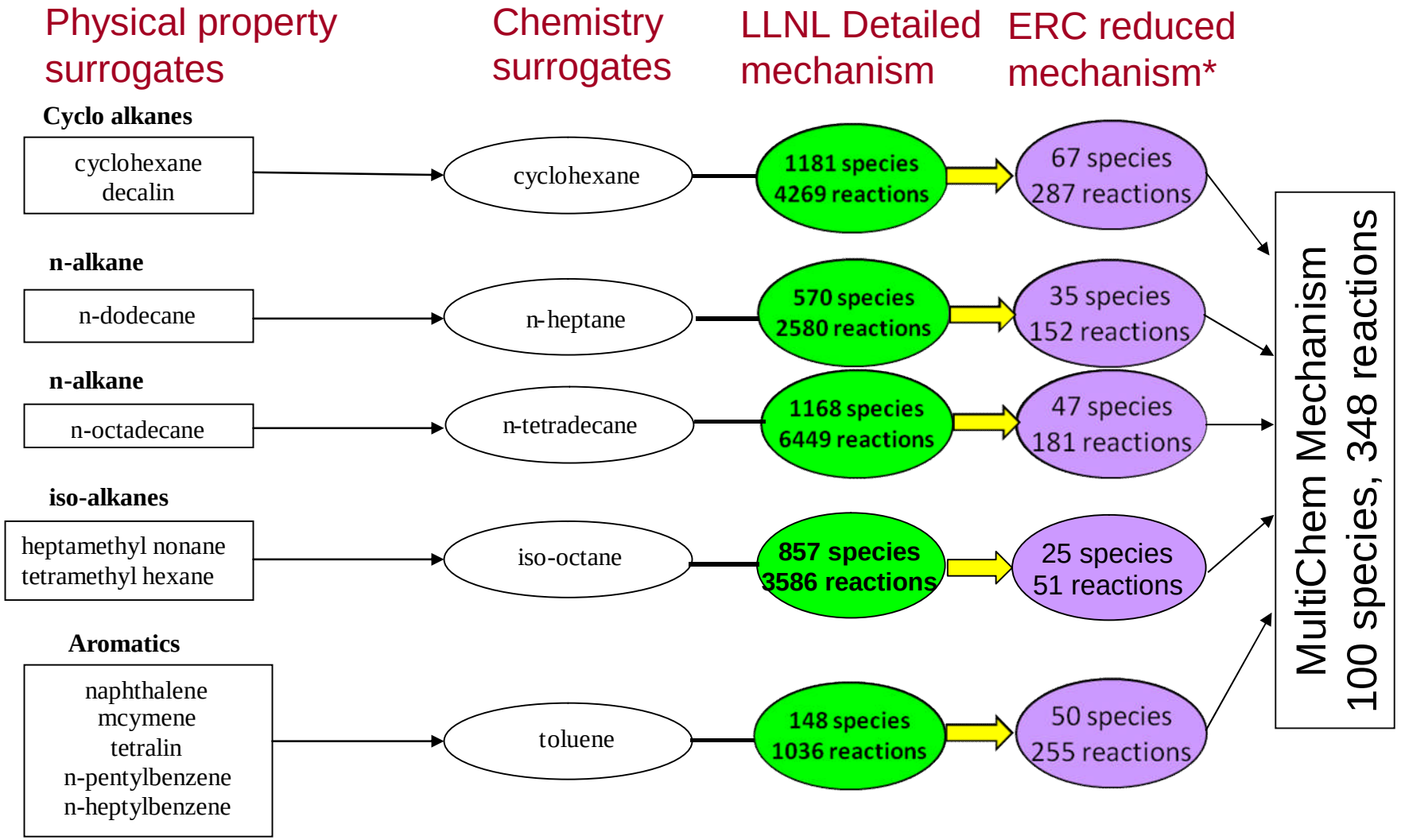






Ra and Reitz, 2008

Chemical class grouping – "MultiChem" skeletal mechanism

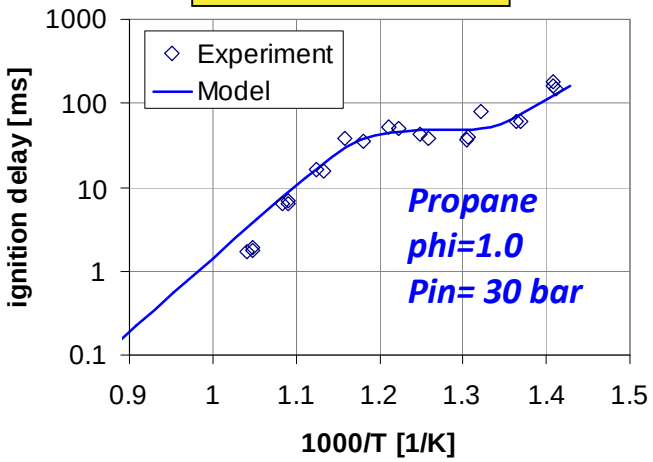


Ra and Reitz, 2011

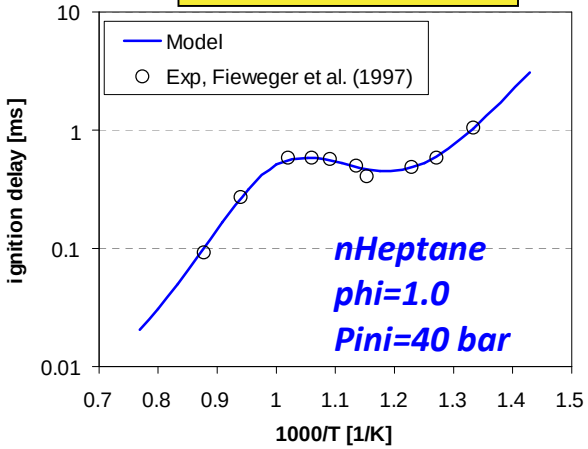
Ignition delay validations of "MultiChem"

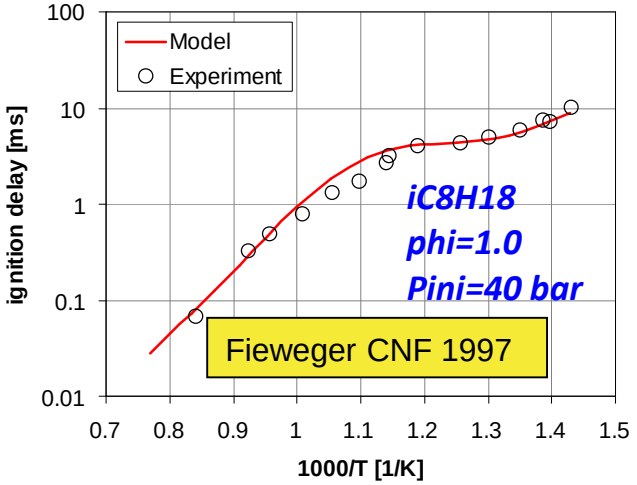
8 Surrogate fuels: *n-heptane, iso-octane, tetradecane, cyclohexane, toluene, decalin, ethanol, MB/D……*

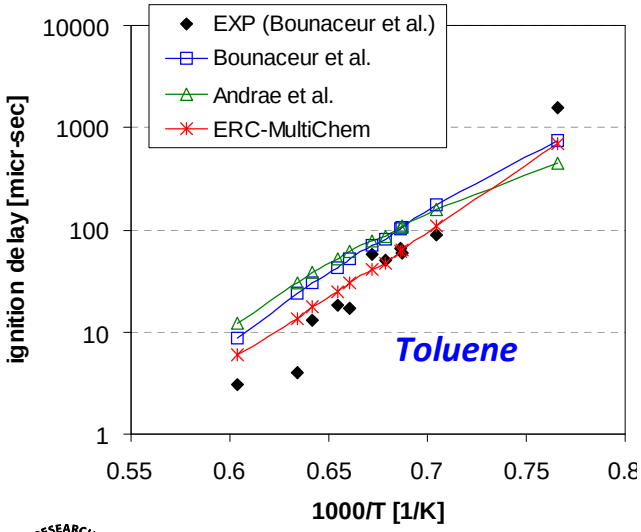
Gauthier CNF 2004



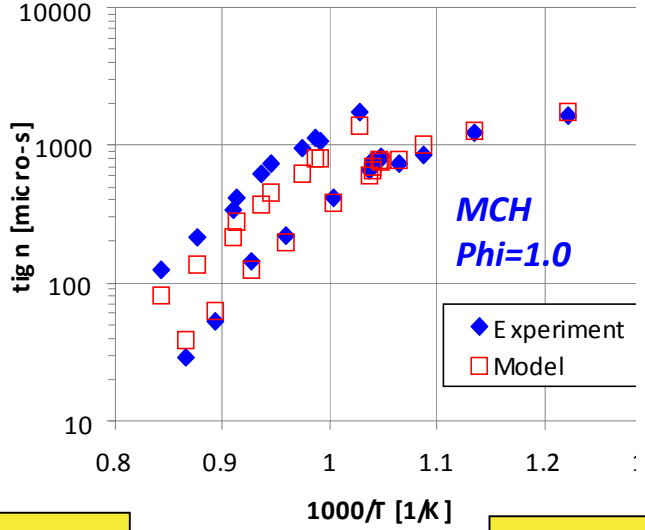
Fieweger CNF 1997

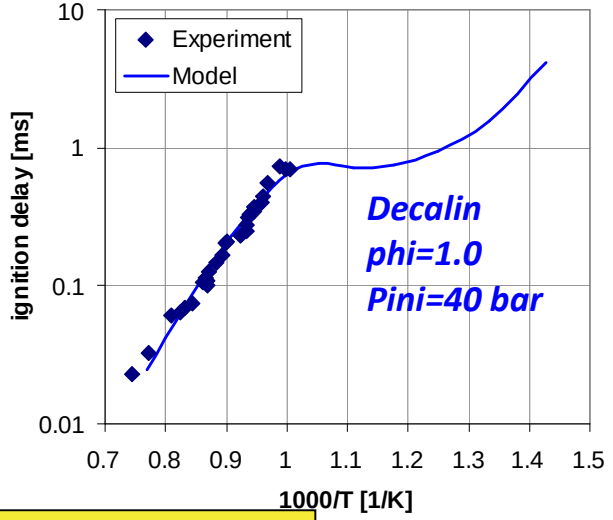






Bounaceur IJCK 2005; Andrae CNF 2005

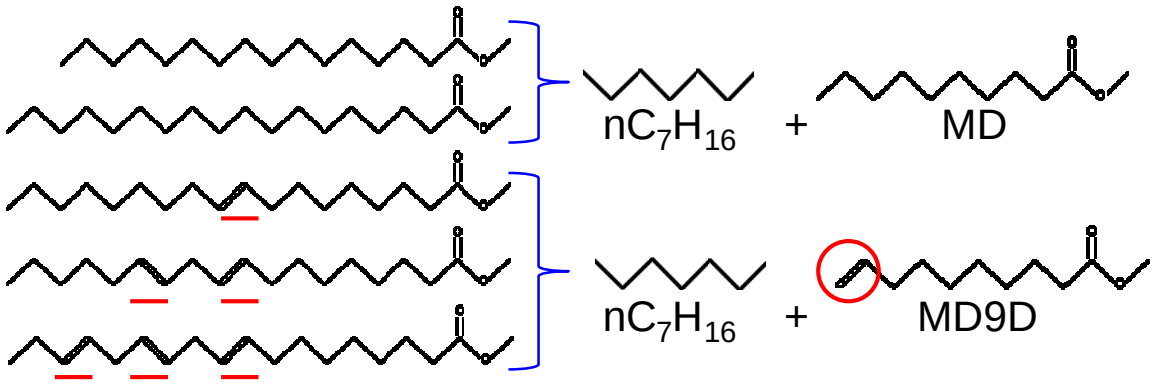




Shen,Energy & Fuels, 2009

Biofuel models – biodiesel and ethanol

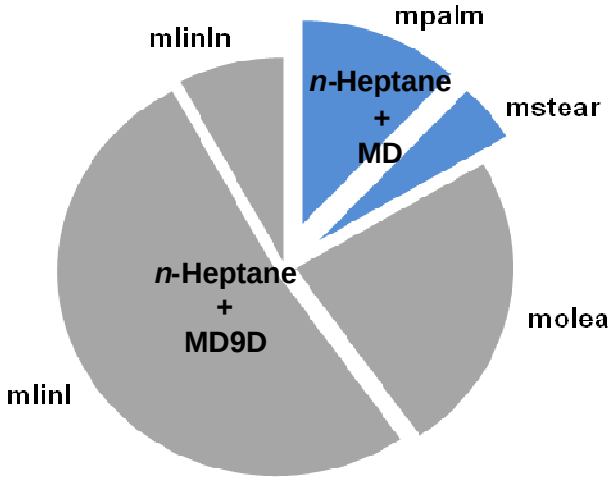
- Soy-based biodiesel:
  - Methyl palmitate (C16:0)
  - Methyl stearate (C18:0)
  - Methyl oleate (C18:1)
  - Methyl linoleate (C18:2)
  - Methyl linolenate (C18:3)

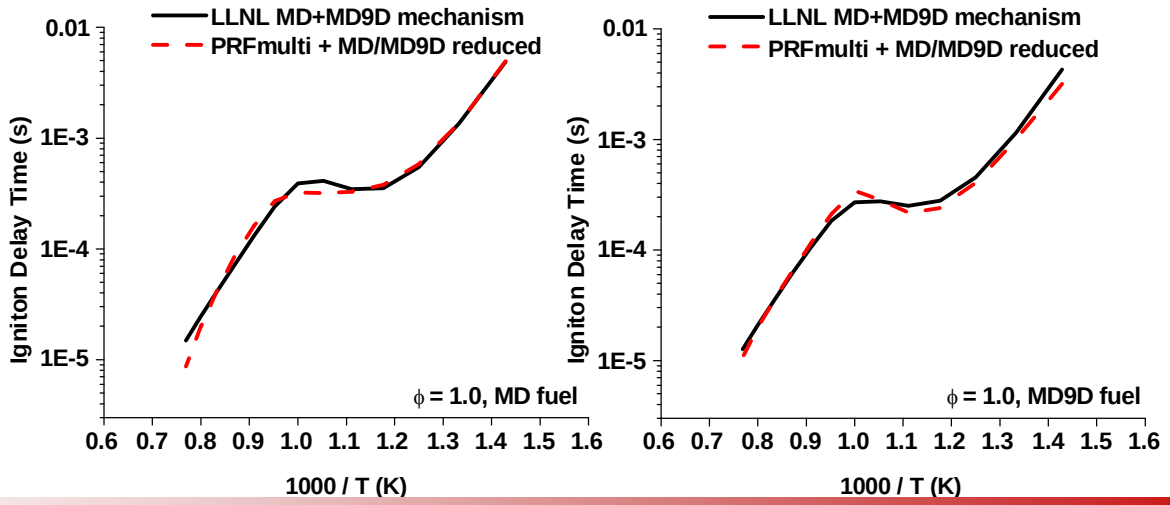


LLNL 3299 species long-chain methyl ester surrogate

Methyl decanoate (MD), Methyl-9-decenoate (MD9D)

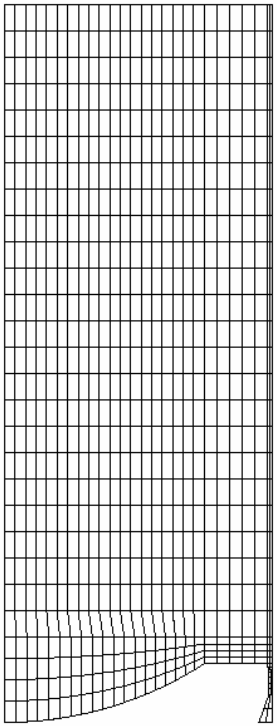
ERC reduced: 85 species



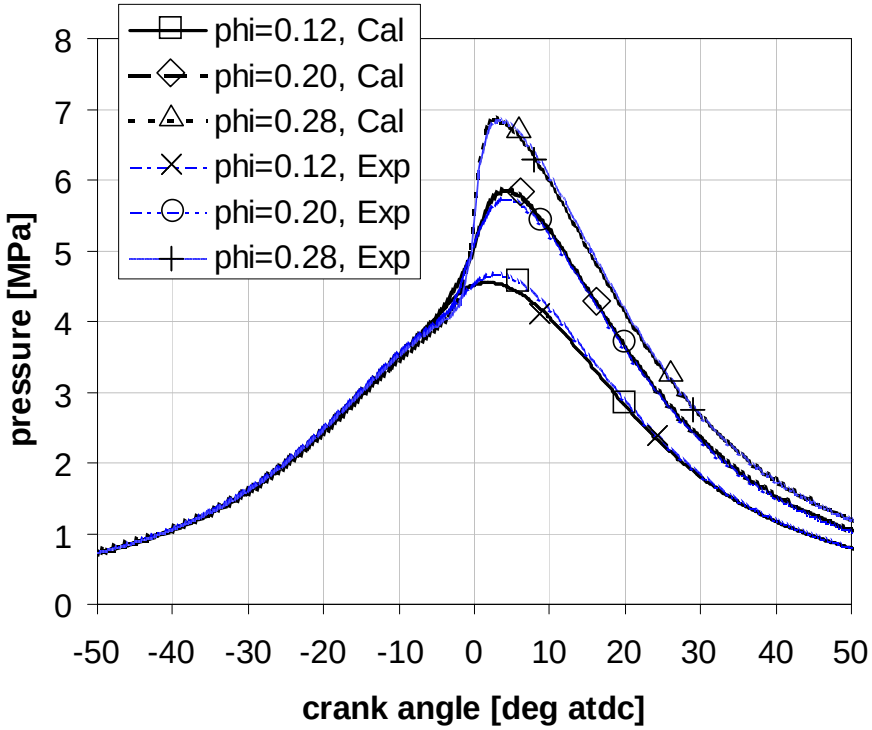


Brakora SAE 2011-01-0831

HCCI Engine validations



2-D grid with 2,734 cells for iso-octane HCCI combustion simulation



Measured and predicted pressure profiles of iso-octane fueled HCCI combustion for various equivalence ratios.

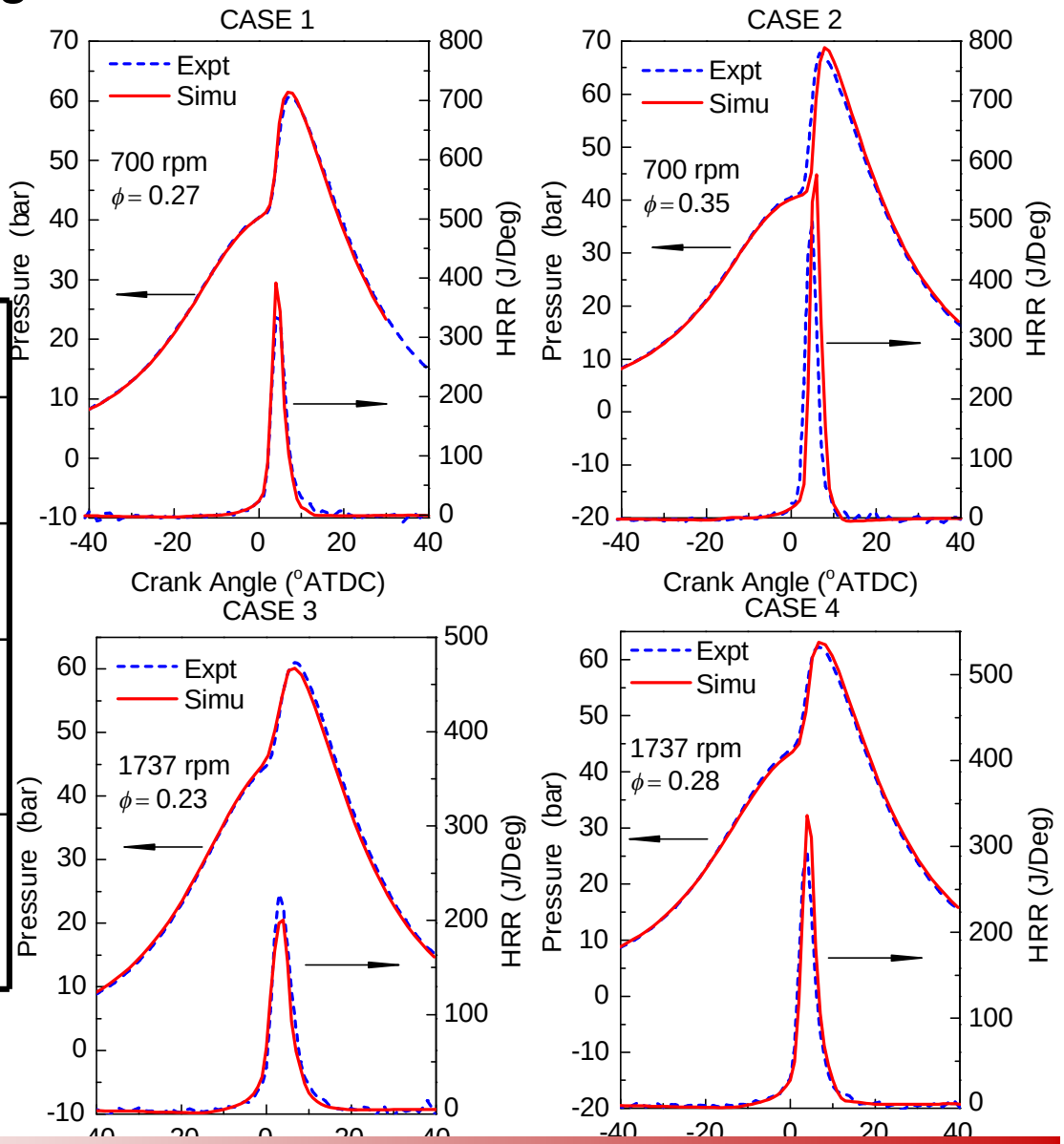
Measured data: Hessel, SAE 2008-01-0047

Ra and Reitz, 2011

Validation - Gasoline HCCI Engine

Caterpillar 3400 engine
Bore = 137.2mm
Stroke = 165.1mm
Compression ratio = 16.1

Cases	1	2	3	4
Engine Speed (rev/min)	700	700	1737	1737
Equivalence Ratio	0.27	0.35	0.23	0.28
Intake Temperature (K)	375	370	400	403
Start of Injection (BTDC)	270	272	304	342



Tamagna, SAE 2007-01-0190

Efficient chemistry solvers

Adaptive multi-grid chemistry (AMC) model

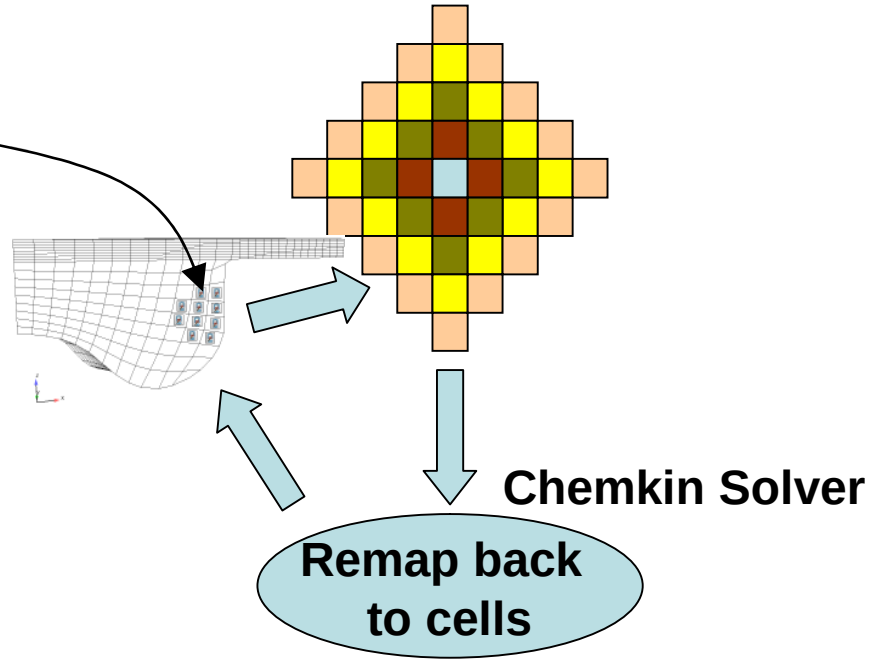
Group thermodynamically-similar cells to reduce the calling frequency to save computer time

Extended dynamic adaptive chemistry (EDAC) scheme Liang, 2009

Dynamically determine the size of fuel chemical mechanism based on the local and instantaneous thermal conditions of the cells

Thermodynamically similar cells (similar temperature, equivalence ratio ϕ)

$$\phi = \frac{2C^{\#}_{-CO_2} + H^{\#}_{-H_2O}/2 - z'C^{\#}_{-CO_2}}{O^{\#}_{-CO_2-H_2O} - z'C^{\#}_{-CO_2}}$$

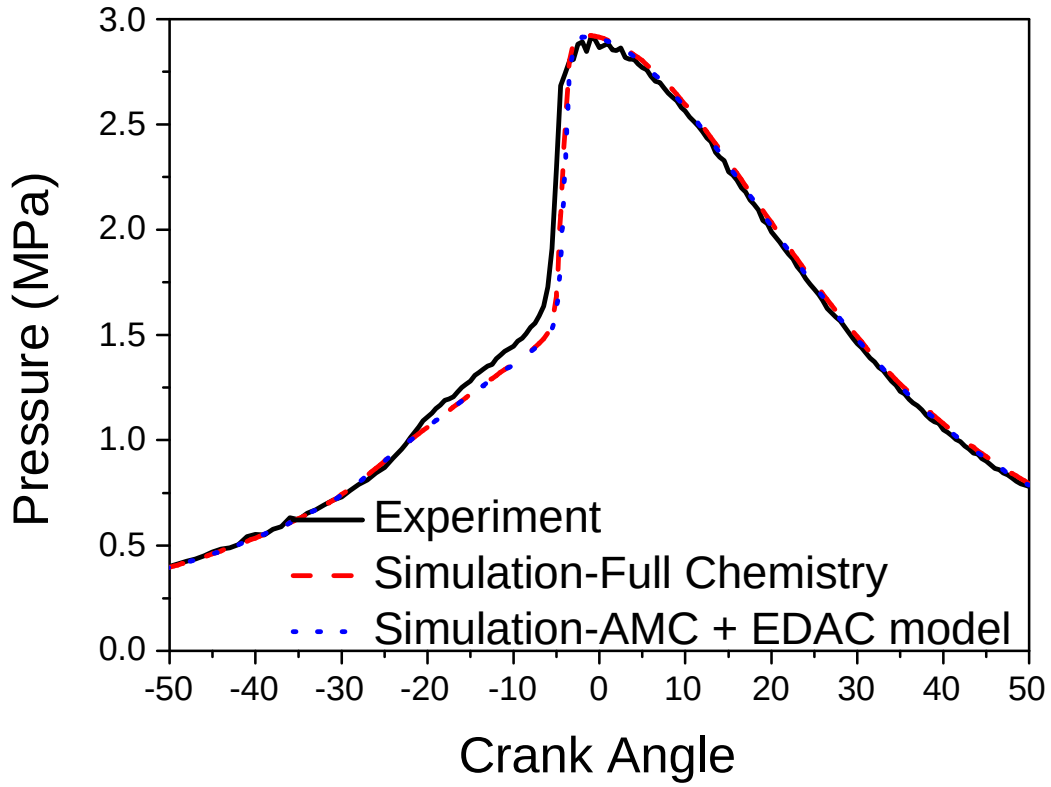


Shi, Ge and Reitz, Springer, 2012

HCCI engine validation

ERC PRF mech.
(39 sp, 141 rxn)

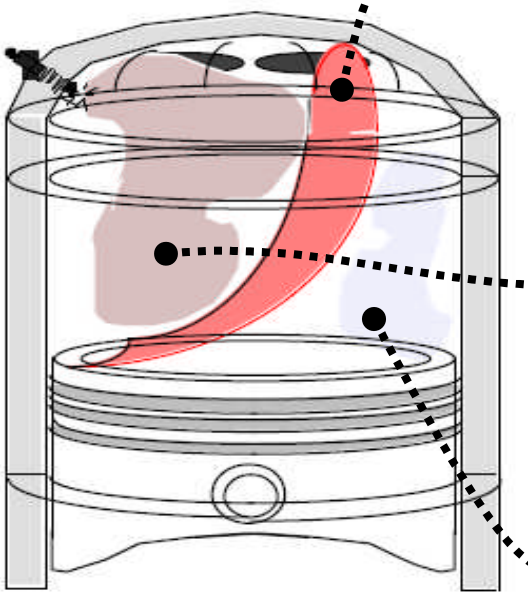
Full	AMC	AMC+EDAC
48.27 hrs.	3.99 hrs.	2.88 hrs.



Shi, Ge and Reitz, Springer, 2012

Flame propagation Models with Detailed Chemistry

Platform: KIVA3V-*G* CFD code + Detailed Chemistry Solver



Spark Ignition Engine

Turbulent Flame Propagation

- *G*-equation description of combustion
- Laminar and turbulent flame speeds
- Primary heat release calculation
- Flame quench due to mixture stratification

Post-flame Chemistry

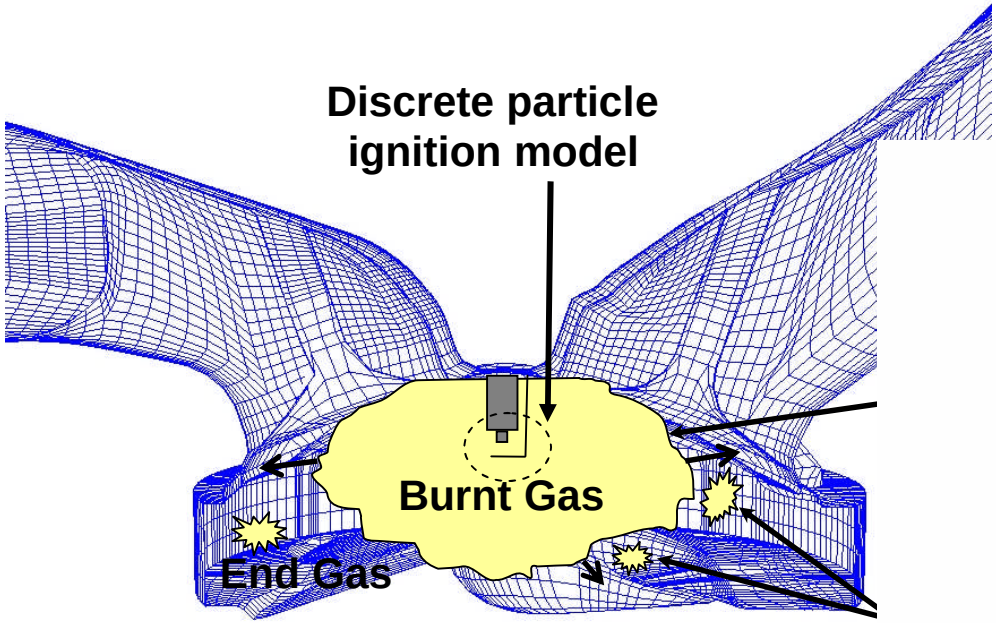
- CO oxidation, H_2-O_2 reactions
- Pollutant formation mechanisms

Knocking Combustion

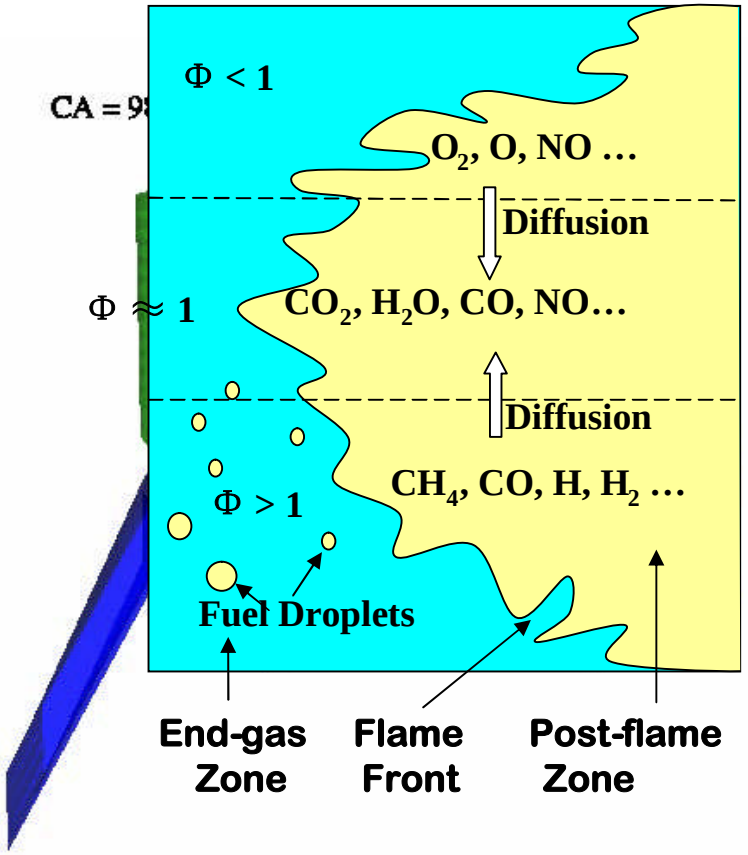
- Auto-ignition mechanisms
- Location / intensity

Liang and Reitz, SAE 2006-01-0243

Ignition and Level set (G-equation) Models



Partially Premixed Flame (DI Engine)



S_T from flame speed correlations

Burned gas: G>0
Unburned gas: G<0

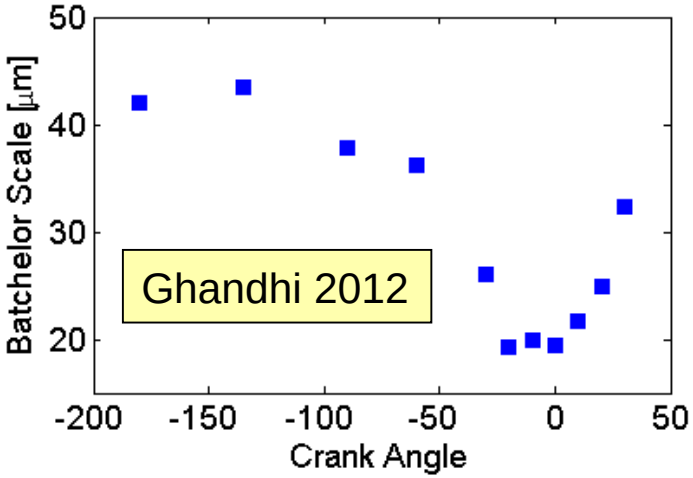
$$\frac{\partial \tilde{G}}{\partial t} + (\vec{v}_f - \vec{v}_{vertex}) \cdot \nabla \tilde{G} = \frac{\overline{\rho}_u}{\overline{\rho}} S_T^0 \left| \nabla \tilde{G} \right| - D_T \tilde{k} \left| \nabla \tilde{G} \right|$$

Liang SAE 2007-01-0165

Turbulent flame structure

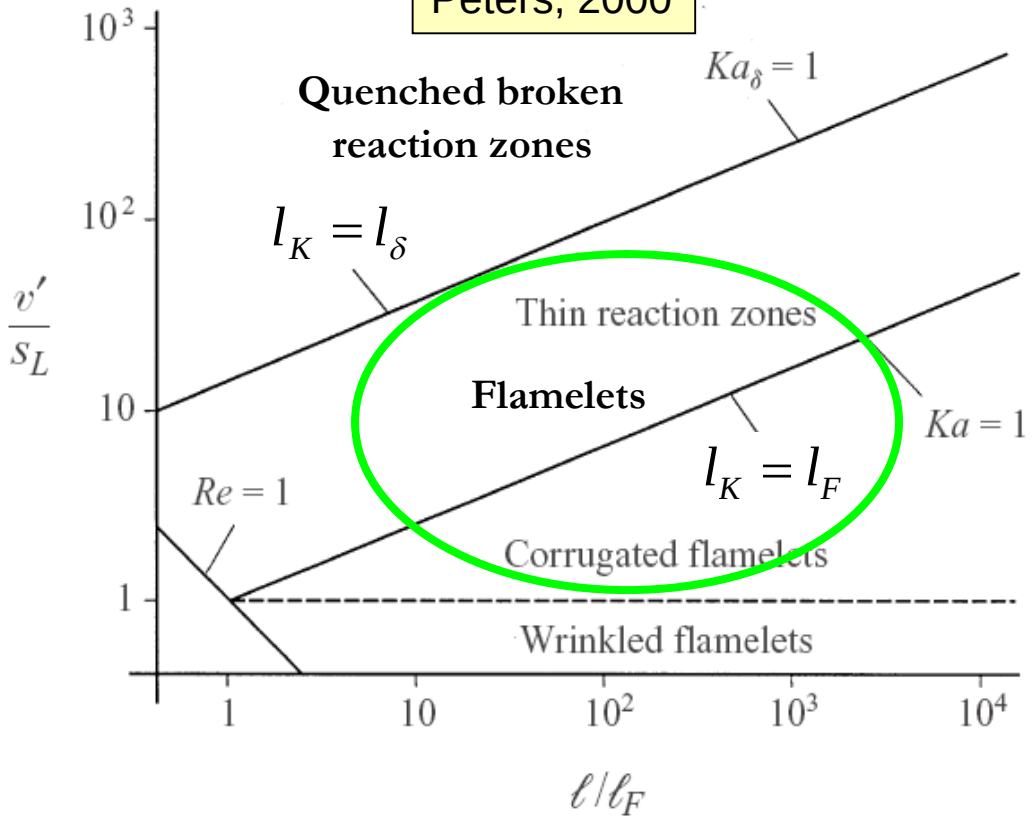
Kolmogorov/Batchelor length scales:

$$l_K = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} = \mathrm{Re}^{-3/4} l_I$$



Combustion regime diagram

Peters, 2000



Laminar flame thickness:

$$l_F = \frac{\left(\lambda / c_p\right)|_{T_0}}{\rho_u S_L} \sim 20\ \mu\mathrm{m}$$

If $l_K < C_{m3} l_\delta = C_{m3} 0.1 l_F$, local $S_T^0 = 0$

Liang SAE 2007-01-0165

It is not possible to resolve a turbulent flame on a practical engine simulation grid

Turbulent Flame Speed Correlation

Peters, 2000

$$\frac{S_T}{S_L \cdot I_0} = 1 + \underbrace{\left[1 - \exp\left(-\frac{C_{m2}\cdot\left(t - t_{ign}\right)}{\tau}\right)\right]^{1/2}}_{\text{Progress Term}} \cdot \left\{-\frac{a_4 b_3^{\,2}}{2b_1}\frac{l}{l_F} + \left[\left(\frac{a_4 b_3^{\,2}}{2b_1}\frac{l}{l_F}\right)^2 + a_4 b_3^{\,2}\frac{u' l}{S_l l_F}\right]^{1/2}\right\}$$

Liang SAE 2007-01-0165

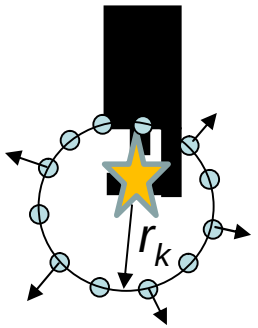
Stretch factor:

$$I_0 = 1 - \underbrace{\left(\frac{l_F}{15\cdot l}\right)^{1/2}\left(\frac{u'}{S_L}\right)^{3/2}}_{\text{Turbulence stretch}} \underbrace{-2\frac{l_F}{r_K}\cdot\frac{\rho_u}{\rho_K}}_{\text{Curvature}}$$

Characteristic Timescale: $\tau = \dfrac{k}{\varepsilon}$

Transition criterion: $r_k \geq C_{m1}\cdot l_I = C_{m1}\cdot 0.16\dfrac{k^{1.5}}{\varepsilon}$

Discrete Particle Ignition Kernel (DPIK) model



Fan & Reitz 2000

$$\frac{\partial \tilde{G}}{\partial t} + (\vec{v}_f - \vec{v}_{vertex})\cdot\nabla\tilde{G} = \frac{\bar{\rho}_u}{\bar{\rho}} S_T^0 \left|\nabla\tilde{G}\right| - D_T\tilde{k}\left|\nabla\tilde{G}\right|$$

Laminar Flame Speed Correlations

Liang SAE 2007-01-0165

Power Law (Metghalchi & Keck, 1982):

$$S_L = S_{L,0}\left(\frac{T}{T_0}\right)^{\alpha}\left(\frac{p}{p_0}\right)^{\beta}\left(1-2.1Y_{dil}\right)$$

$$\alpha = 2.18 - 0.8(\varphi - 1)$$

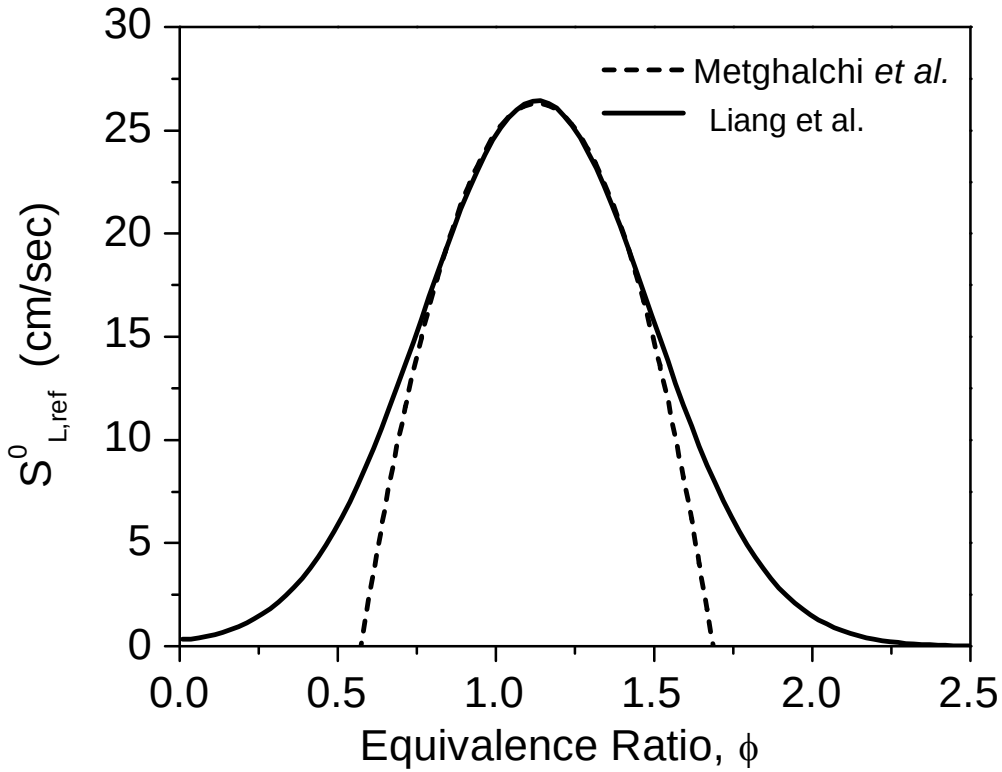
$$\beta = -0.16 + 0.22(\varphi - 1)$$

Reference State: 300K, 1bar

$$S_{L,0} = B_m + B_2(\varphi - \varphi_m)^2$$

Liang et al. :

$$S_{L,0} = \omega\varphi^{\eta}\exp\left(-\xi(\varphi-\sigma)^2\right)$$



For *iso*-octane, $\omega = 26.9$ $\eta = -0.134$ $\xi = 3.86$ $\sigma = 1.146$

Turbulent flame front zone (primary heat release)

Species Production Rate within Flame Containing Cells:

$$\frac{d\rho_i}{dt} = \frac{\rho^u \left(Y_i^b - Y_i^u\right) \cdot A_{i4} \cdot S_T}{V_{i4}}$$

1. Unburned V_u and burnt V_b volumes are tracked
2. Y_i^b is determined by the element potential method
3. ρ_i^b is determined by equation of state of burnt mixture

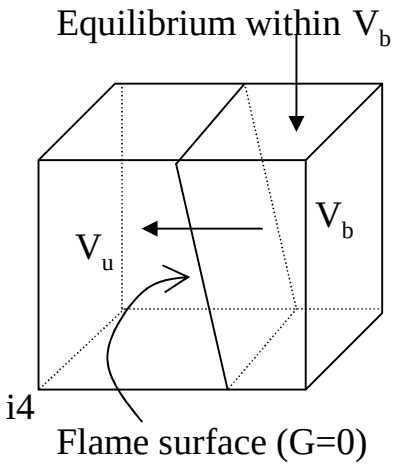
$$\rho_i^b = \rho^b Y_i^b = \frac{p \cdot MW_{mix}^b}{R_u T^b} Y_i^b$$

4. ρ_i^u is determined by mass conservation of species i

$$\rho_i^u = \frac{\rho_i \cdot V_{i4} - \rho_i^b \cdot V^b}{V^u}$$

5. Unburned species mass fractions

$$Y_i^u = \frac{\rho_i^u}{\sum_i \rho_i^u}$$



Liang SAE 2007-01-0165

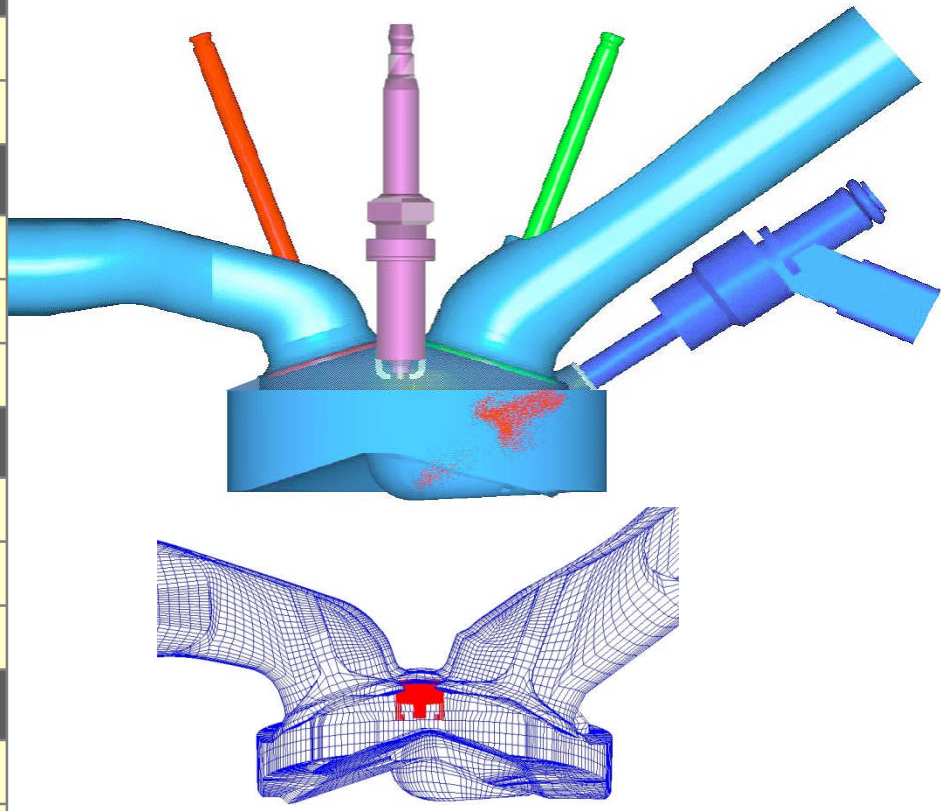
Validation - PFI/DI Gasoline Engine

Liang SAE 2007-01-0165

Bore × Stroke	89 mm × 79.5 mm
Compression Ratio	12 : 1
Engine Speed	1500 rev/min
PFI Mode	
Spark timings (ATDC)	-44, -40, -36, -32
MAP (kPa)	65
DI Mode (Spark timing sweeps)	
Spark timings (ATDC)	-32, -28, -24, -20
MAP (kPa)	75
End of Injection (ATDC)	- 72
DI Mode (Manifold-Absolute-Pressure sweeps)	
MAP (kPa)	75, 80, 90, 100
Spark timing (ATDC)	- 33
End of Injection (ATDC)	- 68
DI Mode (End-Of-Injection sweeps)	
End of Injection (ATDC)	-76, -72, -68, -64
MAP (kPa)	75
Spark timing (ATDC)	- 32

Based on MIT PRF Mechanism (25 species, 51 reactions)

Model constants: Cm1=2.0, Cm2=1.0 (Fixed in all cases)

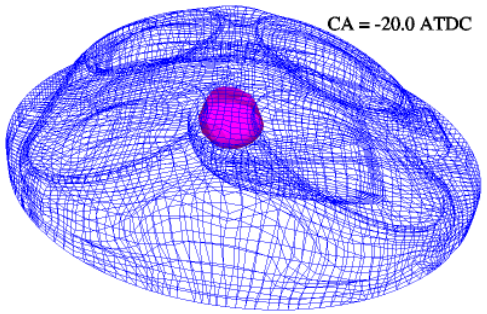


DI Configuration

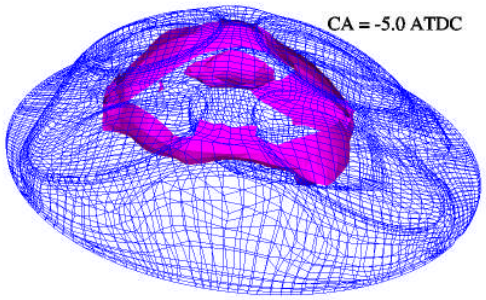
Validation - PFI Engine Operation

Liang SAE 2007-01-0165

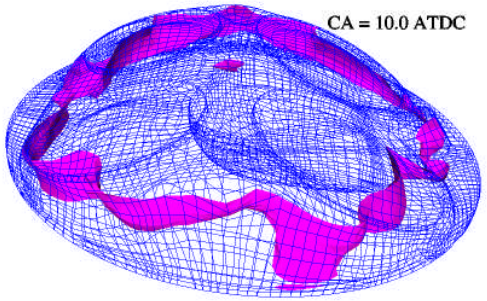
Spark Timing = 40 BTDC



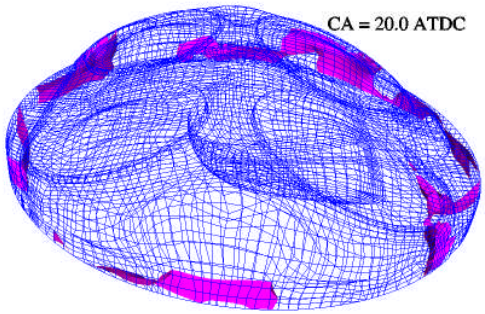
CA = -20 ATDC



CA = -5 ATDC

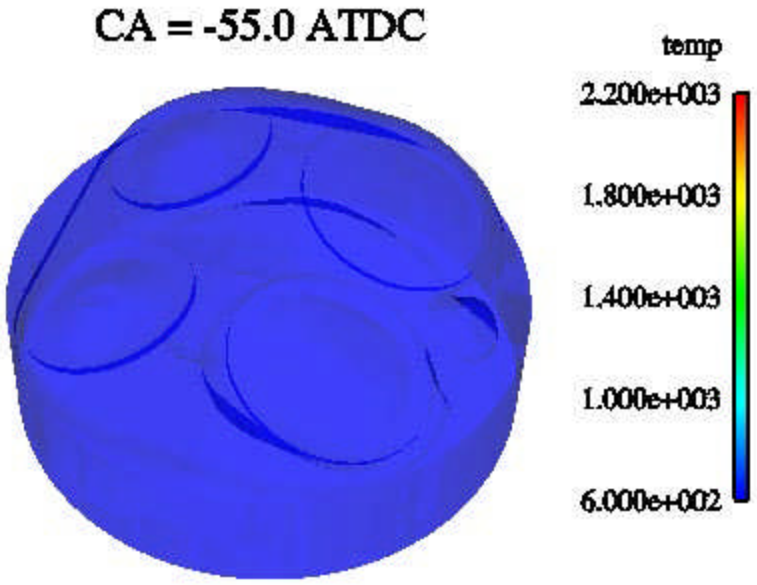


CA = 10 ATDC



CA = 20 ATDC

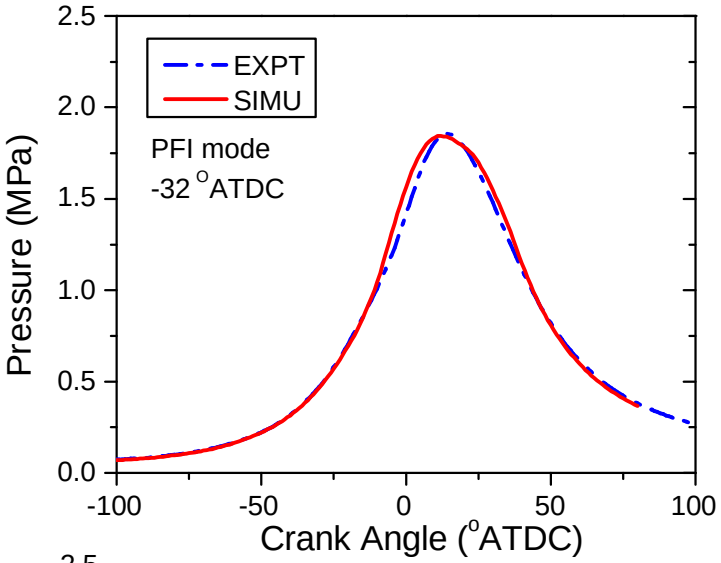
Evolution of the *G*=0 surface

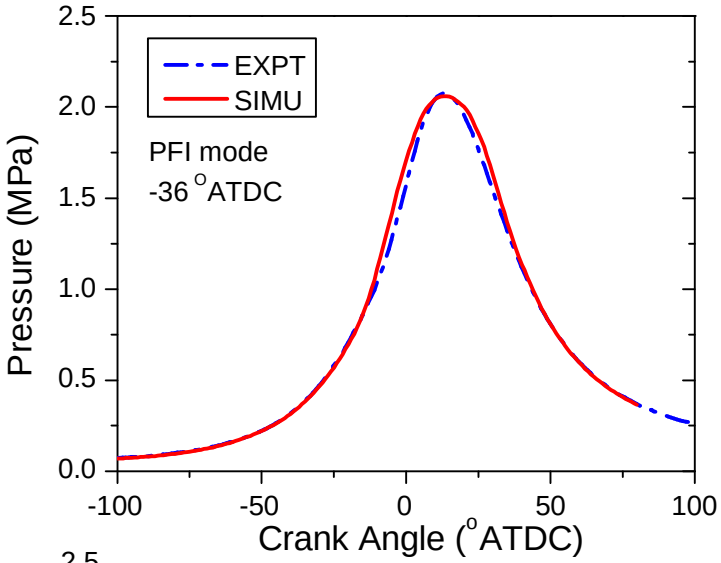


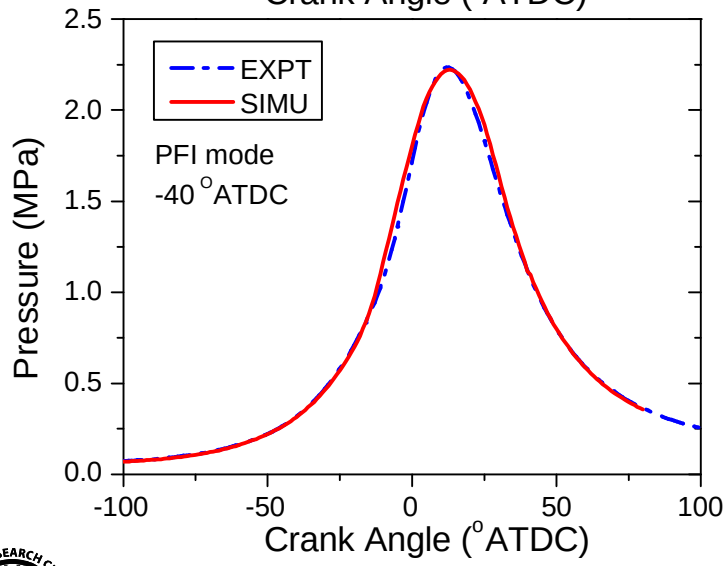
Evolution of Temperature

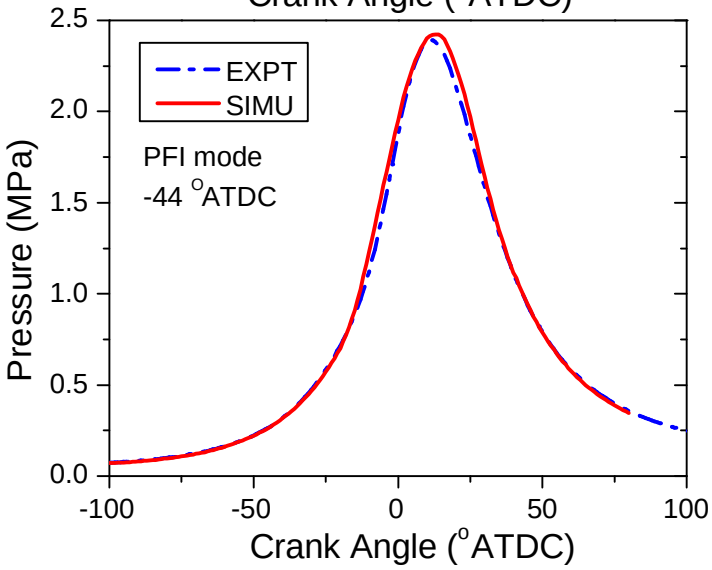
Validation - PFI Engine Operation

Liang SAE 2007-01-0165









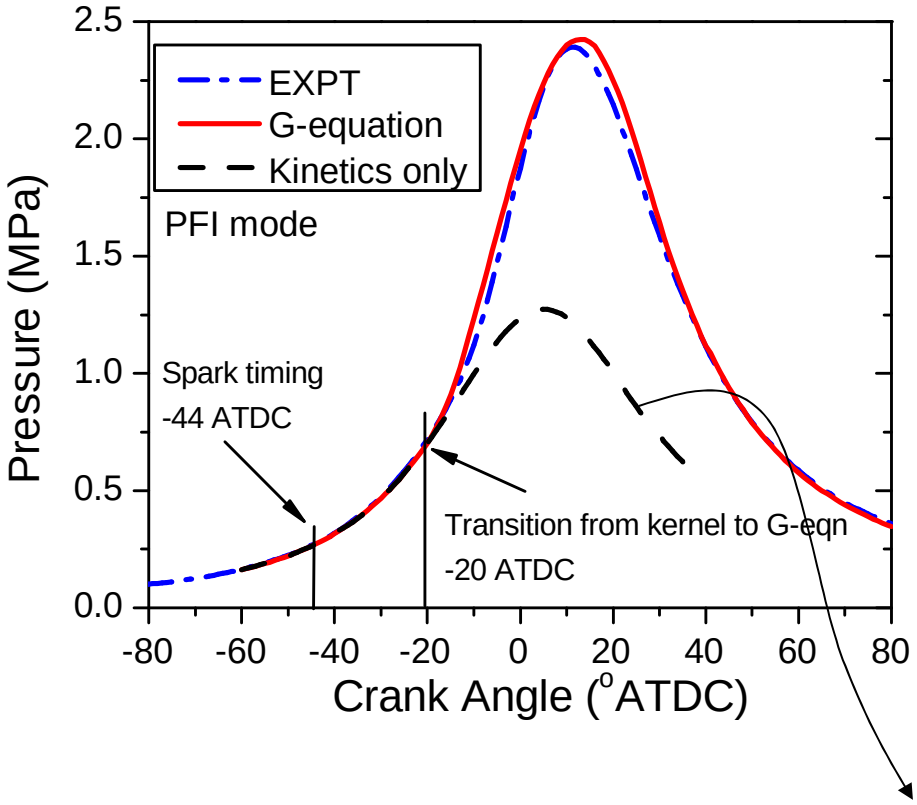
Spark Timing
-44, -40, -36, -32 ATDC
Engine Speed
1500 rpm

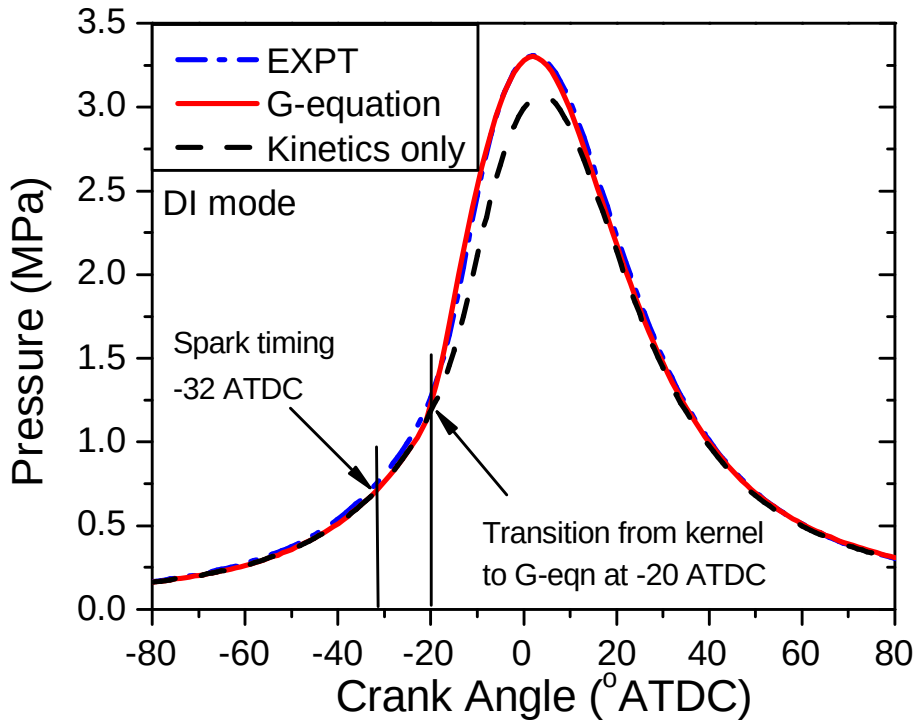
Assessment of the role of flame propagation

Liang SAE 2007-01-0165

Explore Kinetics-Controlled Formulation for Turbulent Flame Propagation:

After ignition kernel stage, each cell is modeled as a WSR, detailed chemistry is applied. "Flame propagation" is controlled by heat conduction and auto-ignition.





Mallard-Le Chatelier propagating wave speed: $S_T = \sqrt{D \frac{dY_i}{dt}}$

Role of flame propagation

PFI case
Spark timing = -44 ATDC

Summary:

Auto-ignition chemistry alone is NOT sufficient to properly model flame propagation.

Turbulence enhancing effect on flame propagation speed in SI engines CANNOT be neglected.

Liang SAE 2007-01-0165