Reciprocating Internal Combustion Engines

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Summer School on Combustion
Course Length: 15 hrs

(Mon.- Fri., June 23 – 27, 2014)

Short course outline:

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)
- Part 1: IC Engine Review, 0, 1 and 3-D modeling
- Part 2: Turbochargers, Engine Performance Metrics

Day 2 (Combustion Modeling)
- Part 3: Chemical Kinetics, HCCI & SI Combustion
- Part 4: Heat transfer, NOx and Soot Emissions

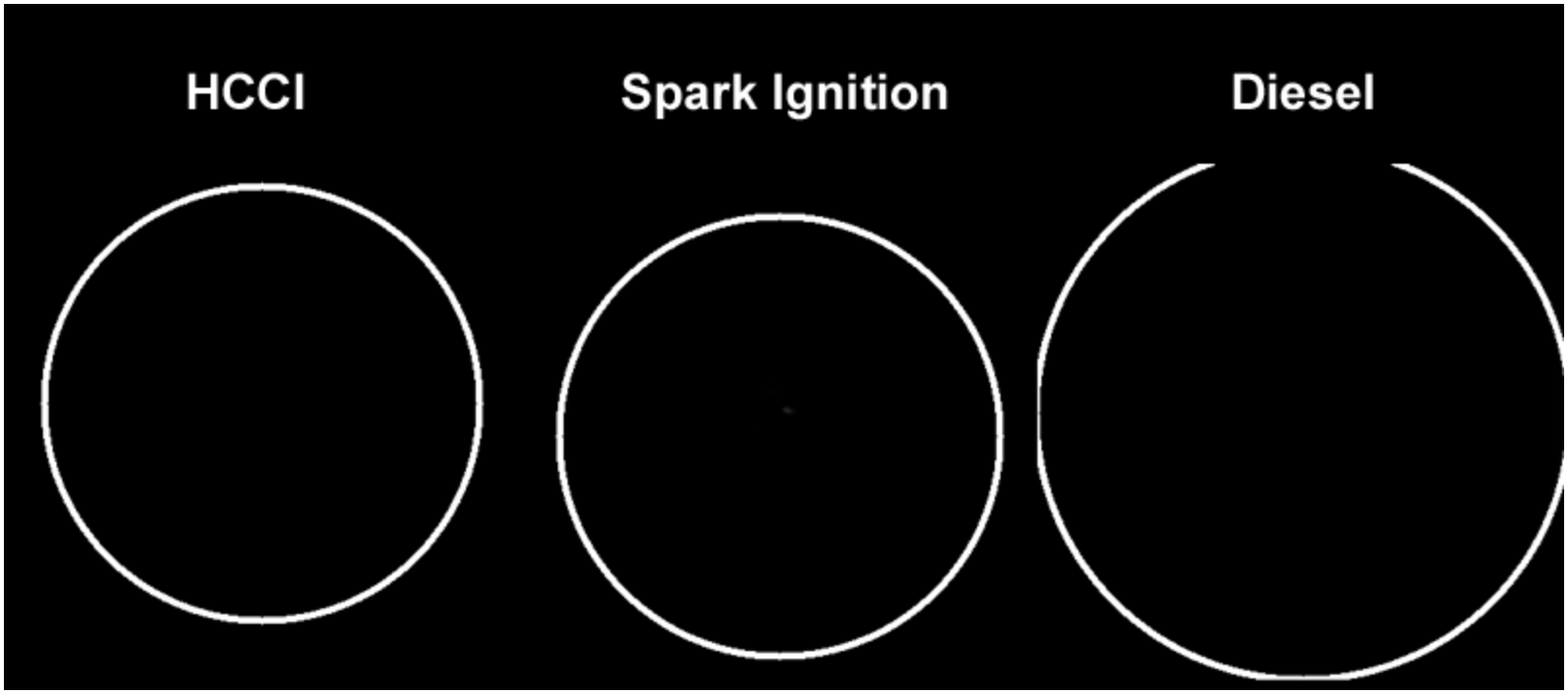
Day 3 (Spray Modeling)
- Part 5: Atomization, Drop Breakup/Coalescence
- Part 6: Drop Drag/Wall Impinge/Vaporization/Sprays

Day 4 (Engine Optimization)
- Part 7: Diesel combustion and SI knock modeling
- Part 8: Optimization and Low Temperature Combustion

Day 5 (Applications and the Future)
- Part 9: Fuels, After-treatment and Controls
- Part 10: Vehicle Applications, Future of IC Engines

Modes of engine combustion

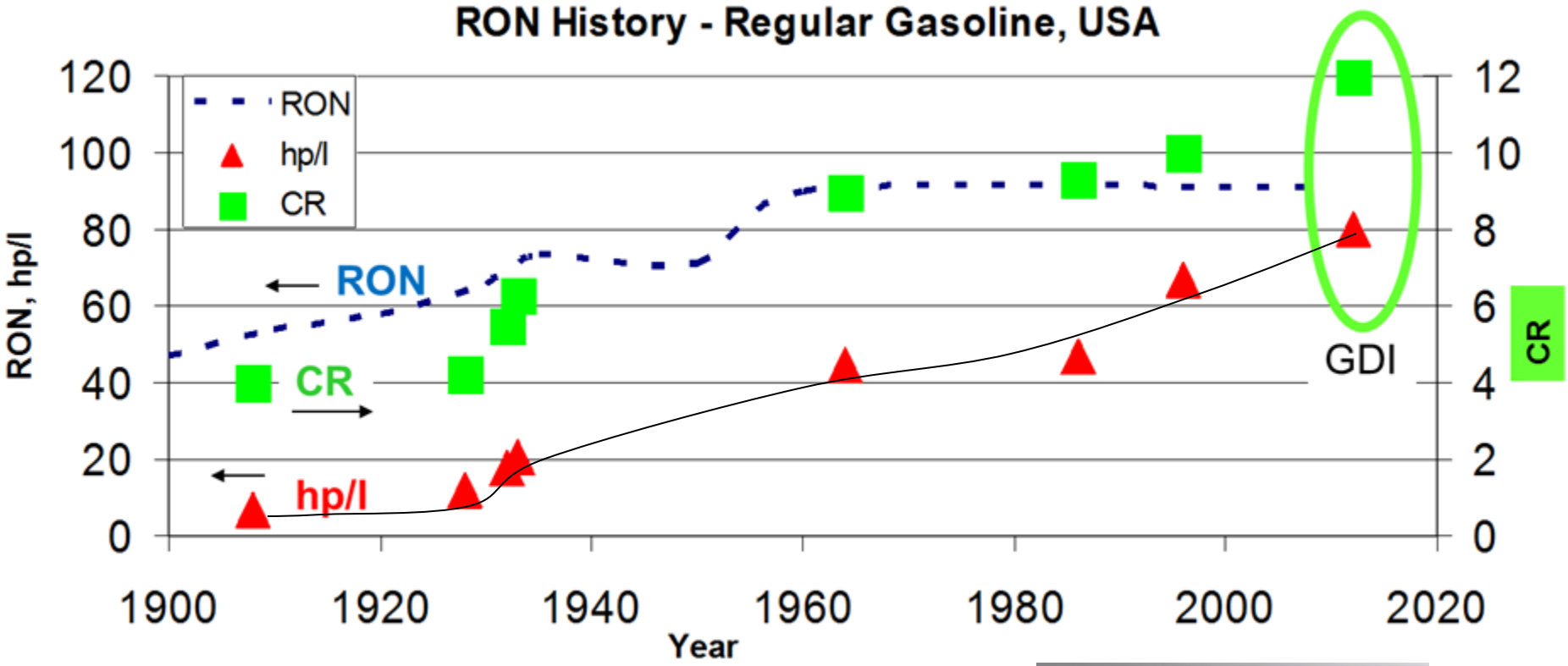
http://www.erc.wisc.edu/combustion.php



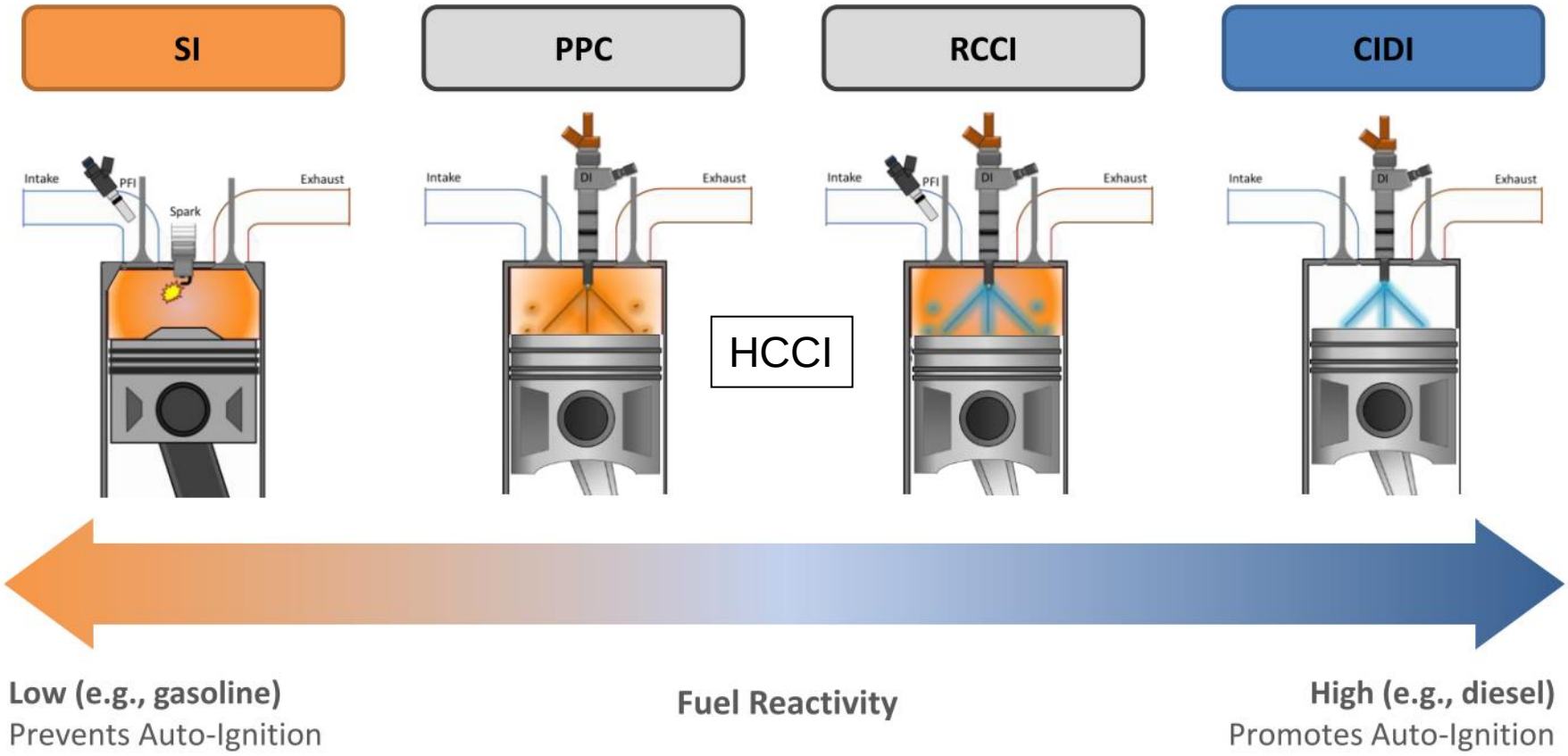
HCCI uses a hybrid combustion strategy. Premixed fuel and air is inducted, but instead of igniting with a spark as in a SI engine, the high temperature from compression causes the mixture to spontaneously react, like in a diesel engine. Ignition occurs at slightly different times at different locations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

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

Chemistry: importance of fuels

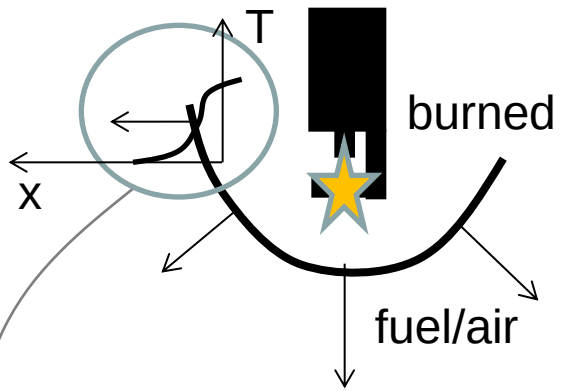


New advanced combustion regimes



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:

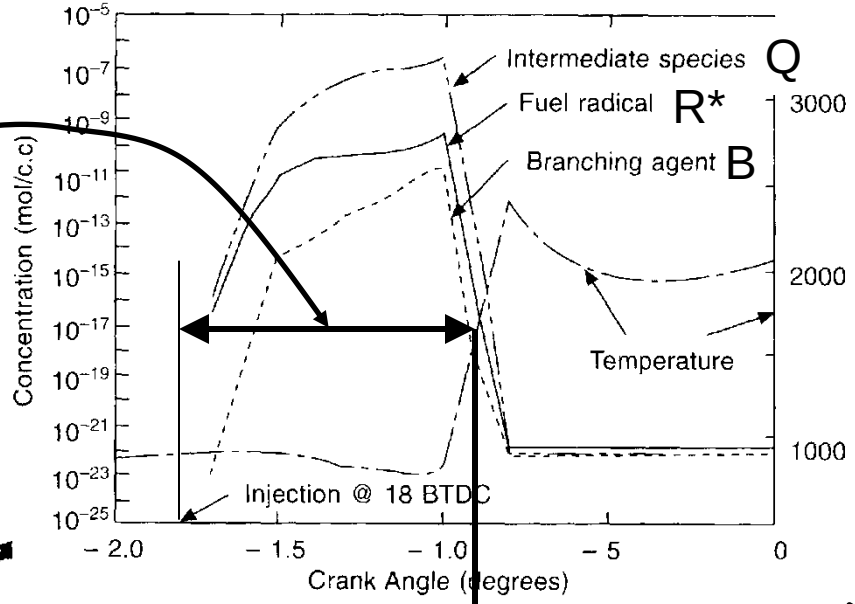
$$S_T = \sqrt{D \frac{dY_i}{dt}} \sim V_{piston}$$

Glassman, 1996

Halstead, 1977

Basic combustion concepts – Diesel (CI)

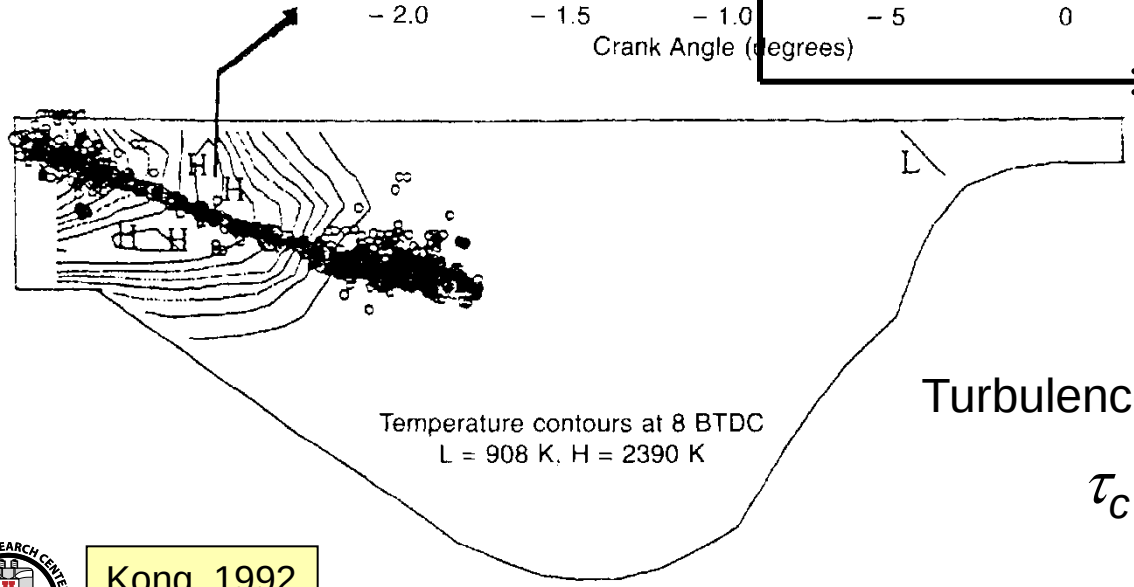
Ignition Delay



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

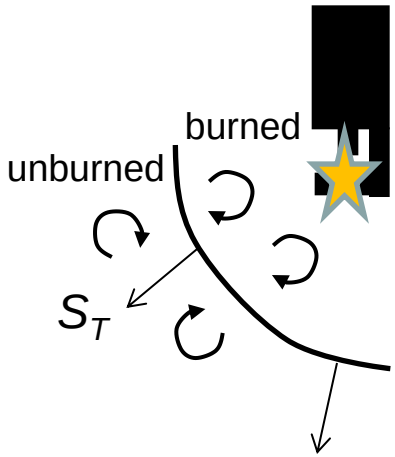
$$\tau_c \sim k/\varepsilon \sim L_{nozzle} / V_{nozzle}$$

Kong, 1992

Turbulent mixing

Spark-ignition

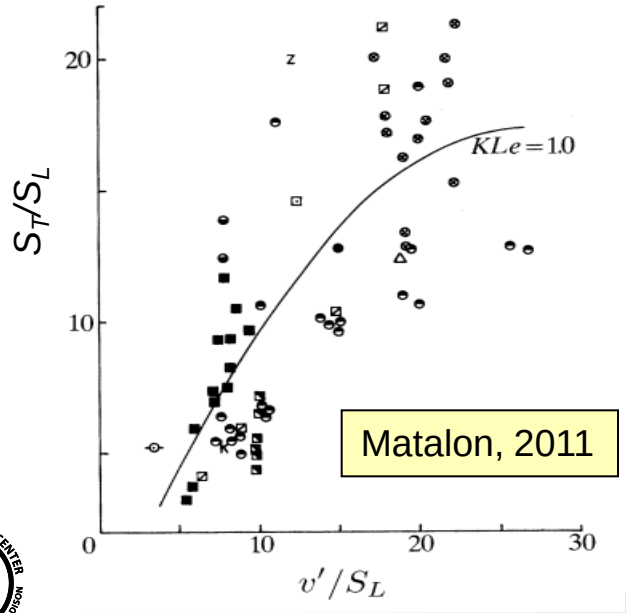
Hot products with
Cold reactants



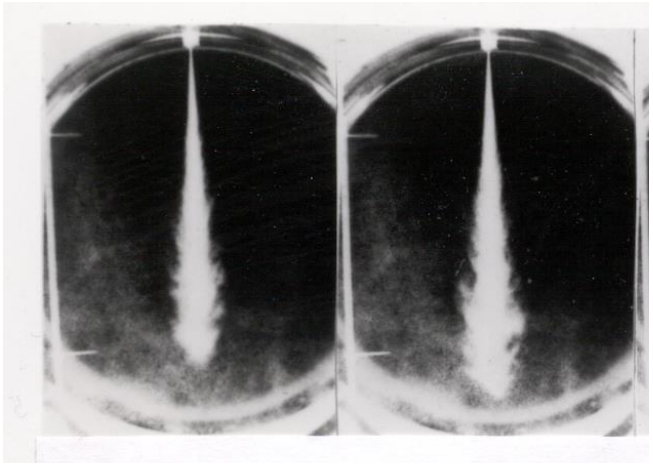
$\tau \sim k/\varepsilon$

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

High turbulence
- faster combustion



Matalon, 2011



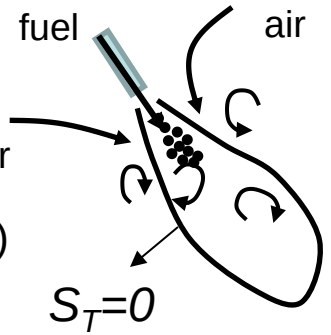
Diesel

Injected fuel with
entrained air

$\tau \sim k/\varepsilon$

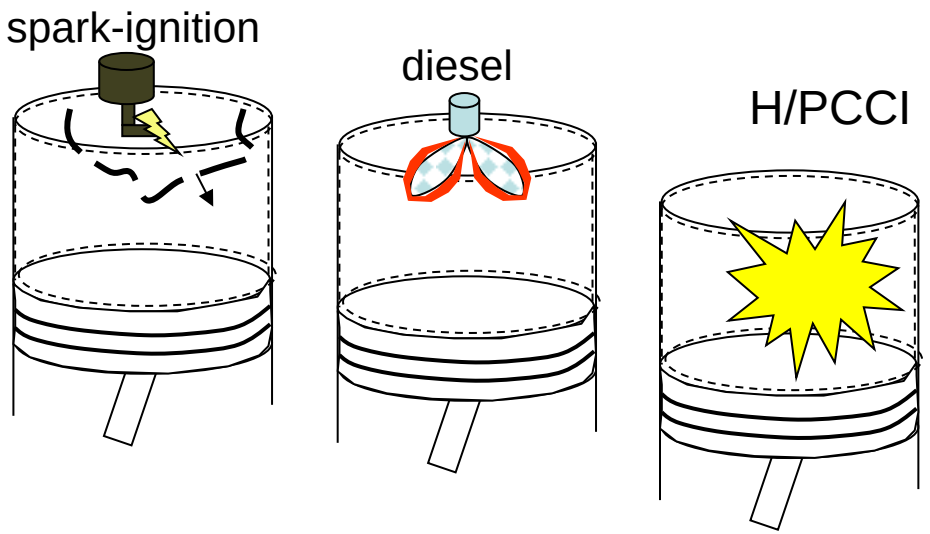
$\sim L_{nozzle} / V_{nozzle}$

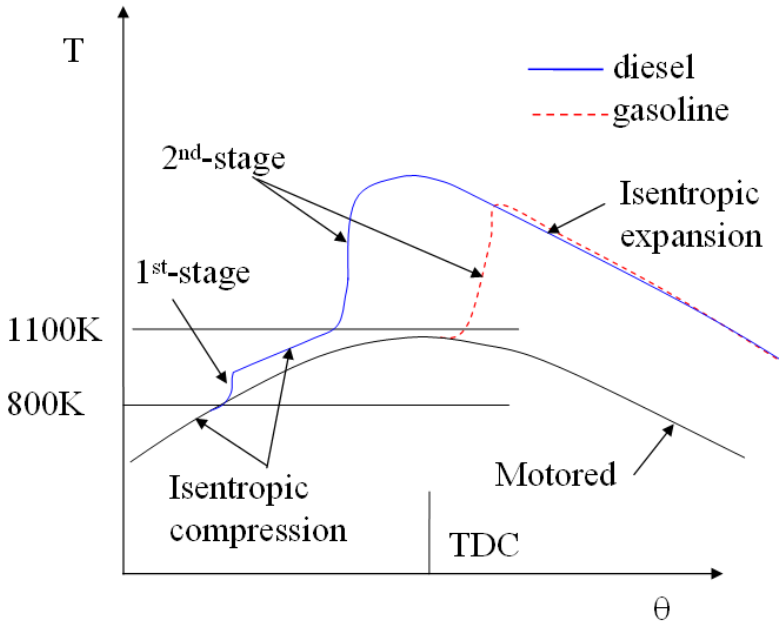
Delayed ignition (PCCI)
- better mixing



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 (CR):
  Sensitive to fuel, poor combustion/load control, low NOx-soot → TE ~50%





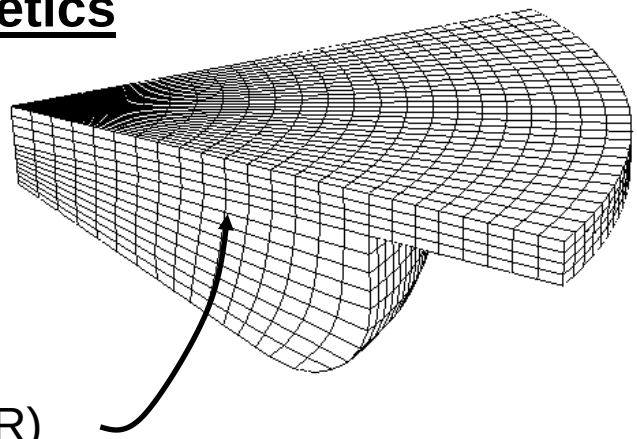
Williams, 1988

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)

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

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

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

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

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

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

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
e_i	species energy

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

Law, 2006

Homogeneous charge: no spatial gradients

$$\frac{\partial Y_i}{\partial t} = \omega_i / \rho$$

$$\frac{\partial T}{\partial t} = -\sum_{i=1}^{n_s} \frac{\Delta h^0_{f,i} \omega_i}{\rho c_p}$$

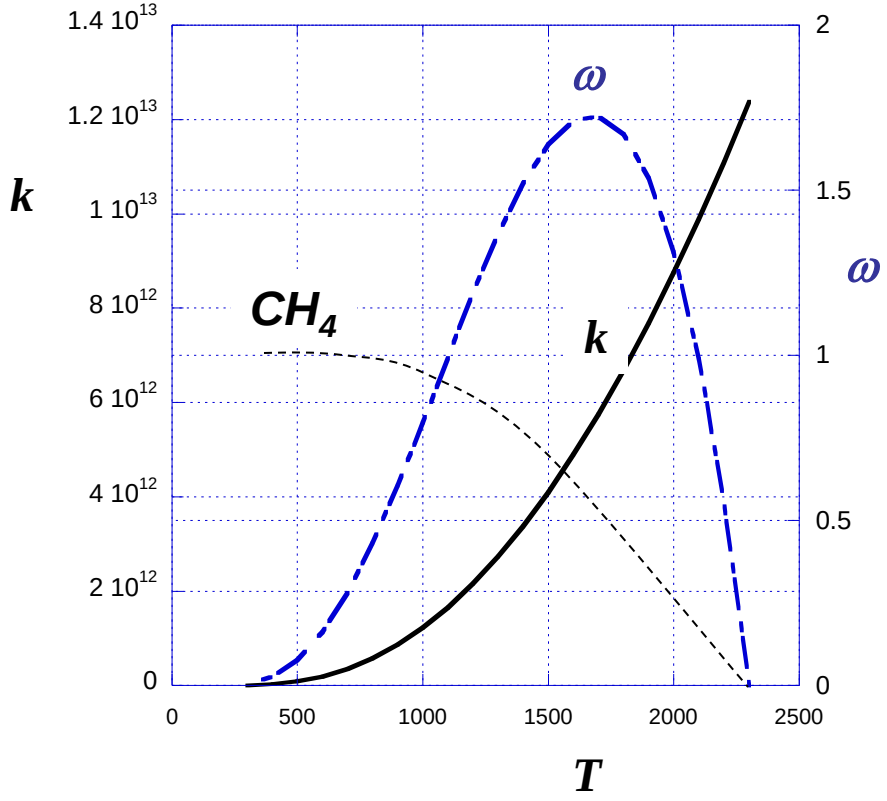
Consider single overall reaction

$$CH_4 + OH \xrightarrow{k} CH_3 + H_2O$$

$$k = AT^b \exp(-E/RT)$$

$$\frac{d[CH_4]}{dt} = -k[CH_4][OH] = \frac{\omega_{CH_4}}{\rho W_{CH_4}}$$

$A = 1.6 \cdot 10^7\ (cm, mol, s),\ b = 1.83,\ E = 11.6\ (kJ/mol)$



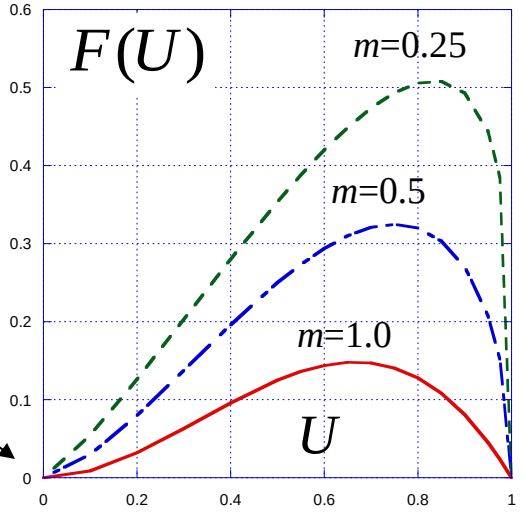
Reitz, 1981

HCCI: Ignition delay

$$\frac{\partial Y_i}{\partial t} = \omega_i / \rho$$

$$\frac{\partial T}{\partial t} = -\sum_{i=1}^{n_s} \frac{\Delta h^0_{f,i} \omega_i}{\rho c_p}$$

Cold boundary difficulty



Consider single component system

$$U = \frac{T - T_{unburned}}{T_{burned} - T_{unburned}}$$

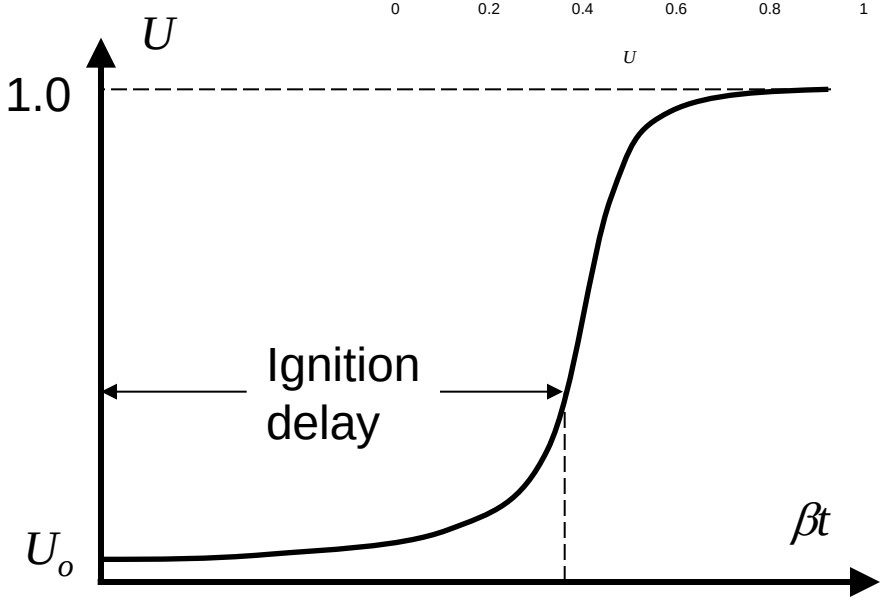
Example:

$$\frac{dU}{dt} = F(U) = \beta U^{m+1}(1-U)^m$$

For $U \rightarrow U_o$: $\quad m\beta t = \frac{1}{U_0^m} - \frac{1}{U^m}$

So, time to reach, say, $5U_0$:

Ignition delay: $\quad \beta t = \frac{4}{5mU_0^m}$



$$m\beta t = Const. - \frac{1}{U^m}\,{}_2F_1(-m, m; (1-m); U)$$

Warnatz, 2006

Combustion chemistry models – CH_4 (15 spec, 31 react.)

$$CH_4 + 2\,O_2 = CO_2 + 2\,H_2O$$

H_2 O_2 chemistry

Hydrogen-Oxygen Chain

1 $H + O_2 \Leftrightarrow OH + O$

2 $H_2 + O \Leftrightarrow OH + H$

3 $H_2 + OH \Leftrightarrow H_2O + H$

4 $H_2O + O \Leftrightarrow 2\,OH$

Hydroperoxyl Formation and Consumption

5[b] $H + O_2 + M \Rightarrow HO_2 + M$

6 $HO_2 + H \Rightarrow 2\,OH$

7 $HO_2 + H \Rightarrow H_2 + O_2$

8 $HO_2 + H \Rightarrow H_2O + O$

9 $HO_2 + OH \Rightarrow O_2 + H_2O$

High temperature

Conversion of Carbon Monoxide to Carbon Dioxide

End

10 $CO + OH \Leftrightarrow CO_2 + H$

Methane Consumption

Start

11 $CH_4 + H \Leftrightarrow H_2 + CH_3$

12 $CH_4 + OH \Rightarrow H_2O + CH_3$

Initiation
H atom abstraction

Methyl Reactions

13 $CH_3 + O \Rightarrow CH_2O + H$

14 $CH_3 + OH \Rightarrow CH_2O + H + H$

15 $CH_3 + OH \Rightarrow CH_2O + H_2$

16[c] $CH_3 + H \Rightarrow CH_4$

23 $CH_3 + H \Rightarrow CH_2 + H_2$

28 $CH_3 + OH \Rightarrow CH_2 + H_2O$

Formaldehyde Reactions

17 $CH_2O + H \Rightarrow CHO + H_2$

18 $CH_2O + OH \Rightarrow CHO + H_2O$

Formyl Reactions

19 $CHO + H \Rightarrow CO + H_2$

20 $CHO + OH \Rightarrow CO + H_2O$

21 $CHO + O_2 \Rightarrow CO + HO_2$

22 $CHO + M \Rightarrow CO + H + M$

Methylidyne Reactions

27 $CH + O_2 \Rightarrow CHO + O$

31 $CH + OH \Rightarrow CH_2O + H$

Methylene Reactions

24 $CH_2 + O_2 \Rightarrow CO_2 + H_2$

25 $CH_2 + O_2 \Rightarrow CO + OH + H$

26 $CH_2 + H \Leftrightarrow CH + H_2$

29 $CH_2 + OH \Rightarrow CH_2O + H$

30 $CH_2 + OH \Rightarrow CH + H_2O$

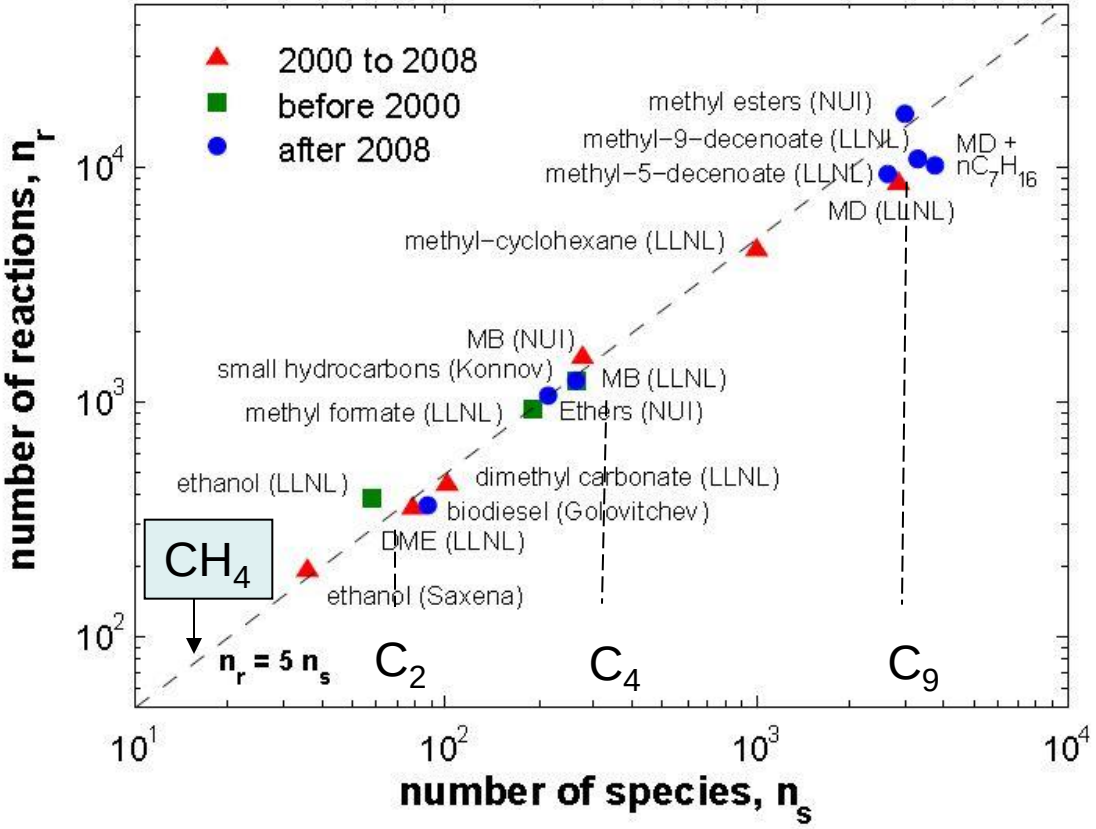
Conversion to products by sequential fragmentation by H abstraction

Lu, 2009
Brakora, 2013

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)

Warnatz, 2006

Hydrocarbon kinetics - NTC

Second Stage Ignition

$H_2O_2 = OH + OH$

RH

O_2

$R^\bullet$

olefin + R

O_2

deceleration

acceleration

RO_2

QOOH

olefin + HO_2

cyclic ether + OH

O_2

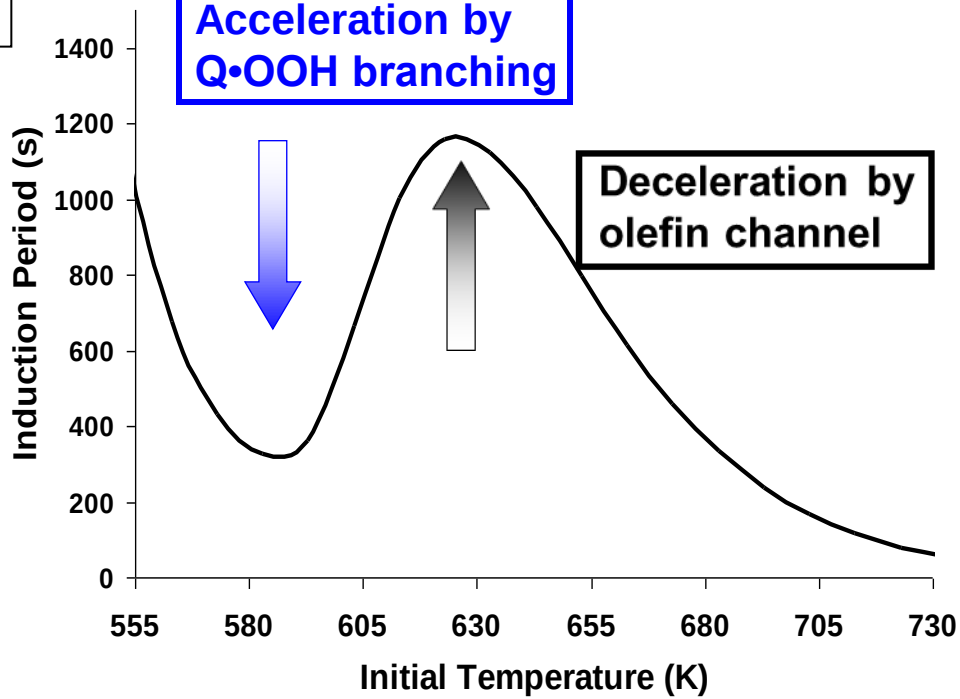
O_2QOOH

keto-hydroperoxide + OH

(low T branching)

Acceleration by Q•OOH branching

Deceleration by olefin channel



First Stage Ignition

Isomerization steps

Warnatz, 2006

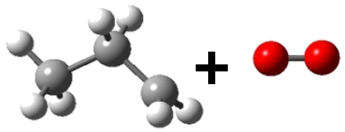
Alkane fuel oxidation

Example: Propane

Fuel: RH → R•

+OH, H,…

n-C_3H_7• + O_2



Smaller R → HCO
CH_3, C_2H_5,…

β-scission

Energy release
CO + OH → CO2 + H

Chain branching
H + O_2 → OH + O

Thermal decomposition
H_2O_2 ↔ OH + OH

Internal H atom abstraction

ROO → QOOH

Chain propagation
QO + OH
Olefin channel

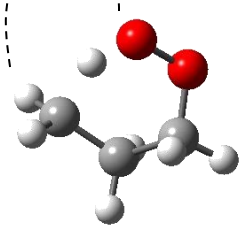
+O_2

OOQOOH

Internal H atom abstraction

HOOQ'OOH

Chain branching
HOOQ'O + OH
↓
OQ'O + OH



•$CH_2CH_2CH_2OOH$

Isomerization

High temperature reaction >1200K

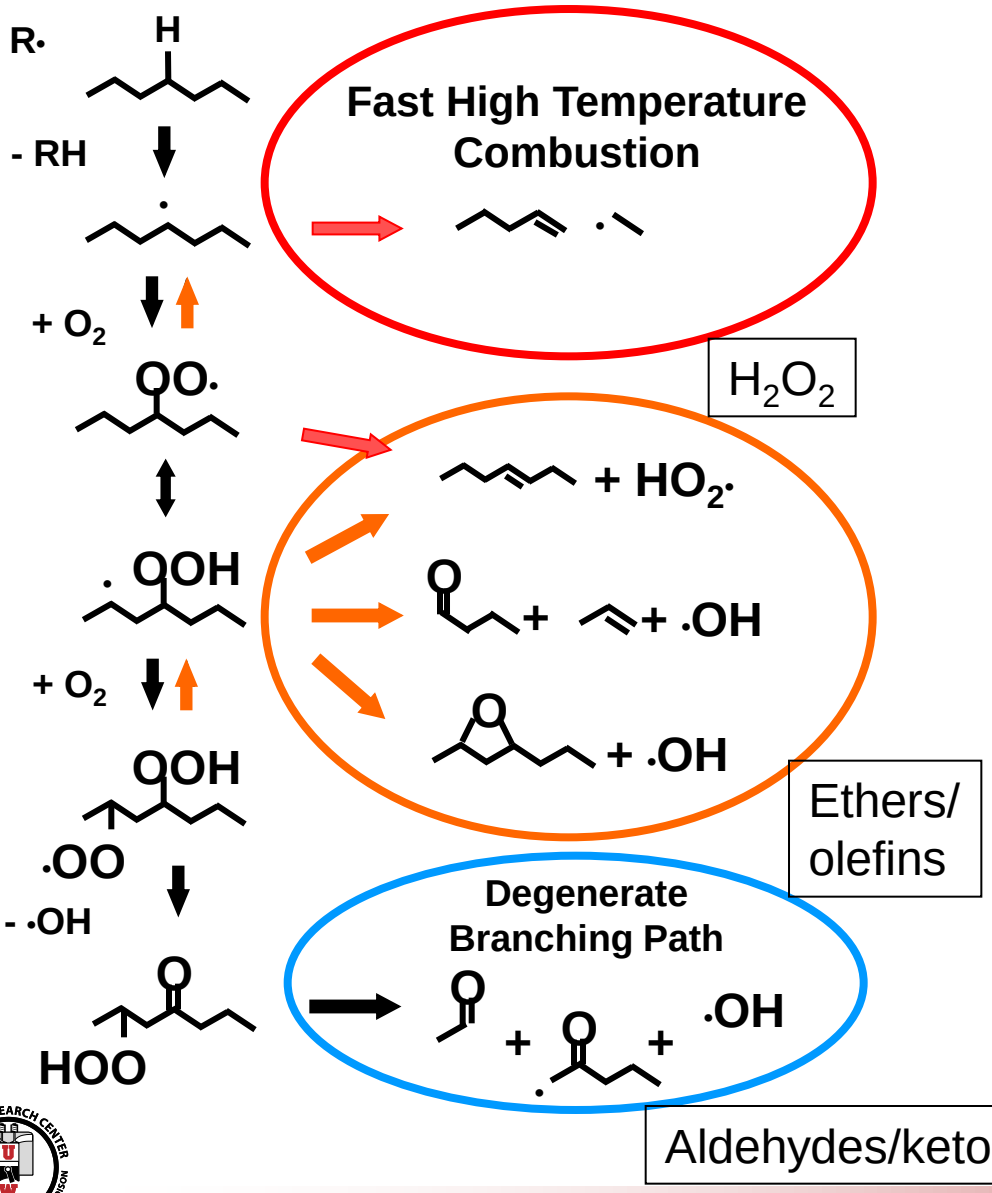
Blue flame 1100K

Negative temperature coefficient 800 ~900K

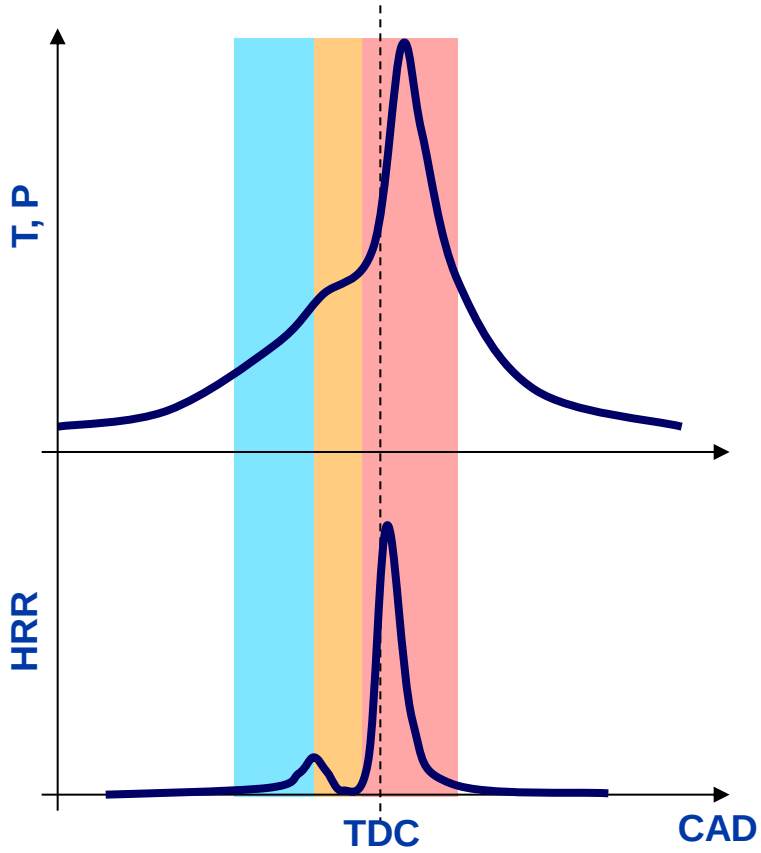
Cool flames 800K

Mehl, 2009

HCCI combustion kinetics

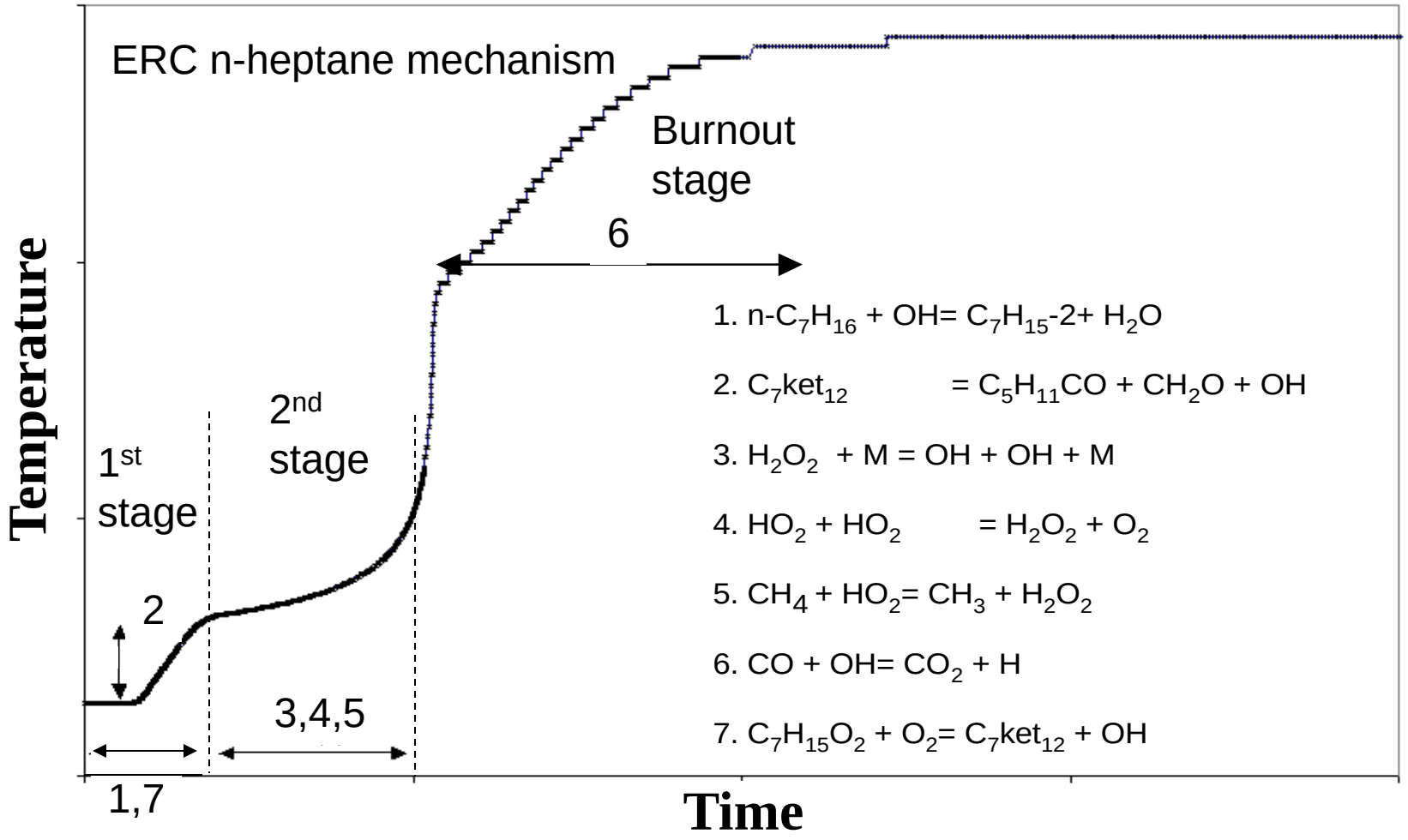


Typical HCCI Combustion Temperature and Heat Release Rate profiles



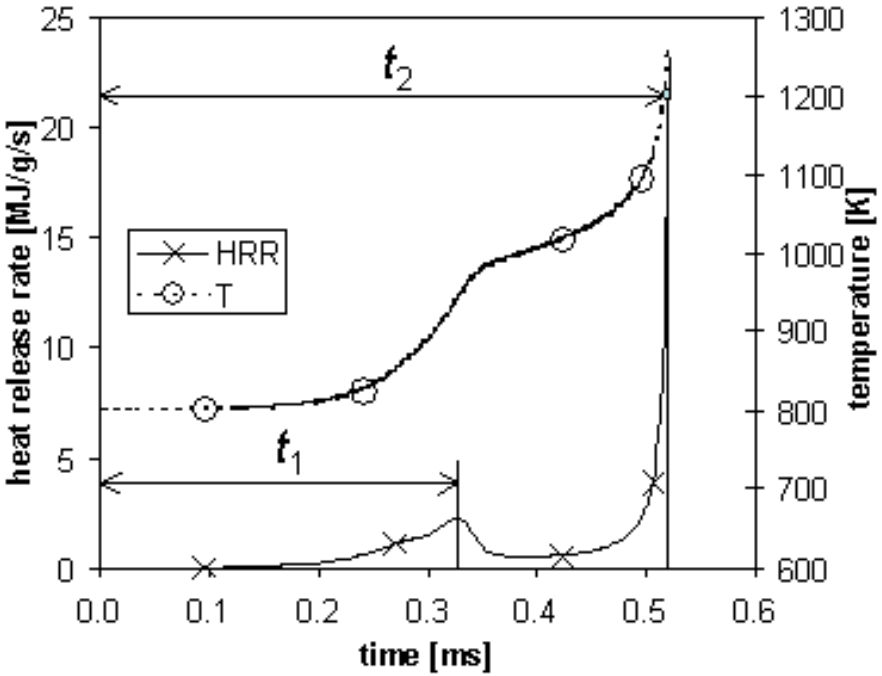
Patel, 2004

Mechanism reduction – identify key reaction steps



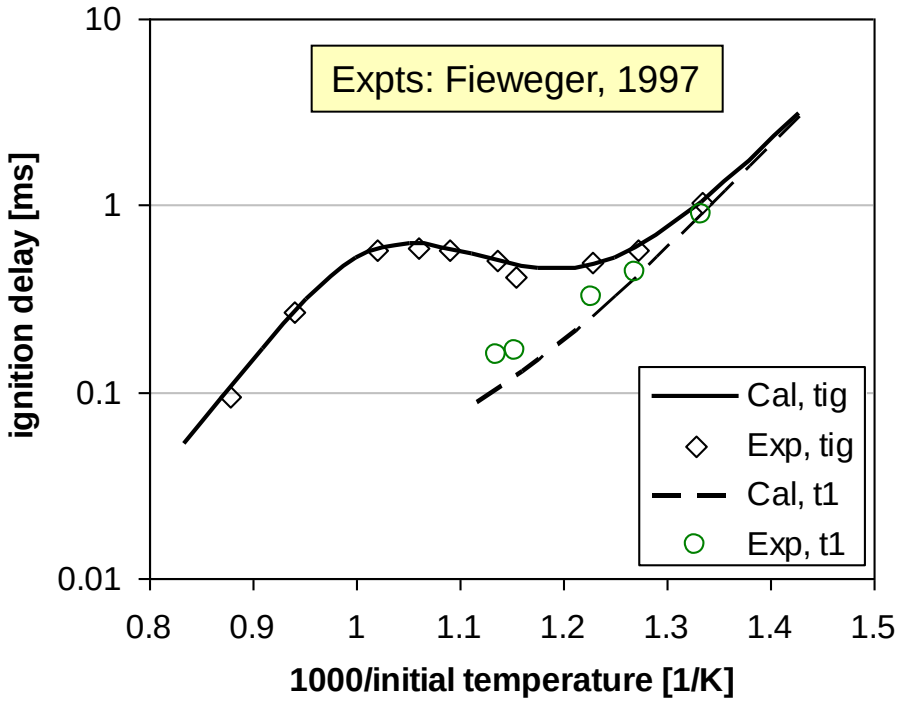
Ra, 2008

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



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: $A = k \times A_{base}$

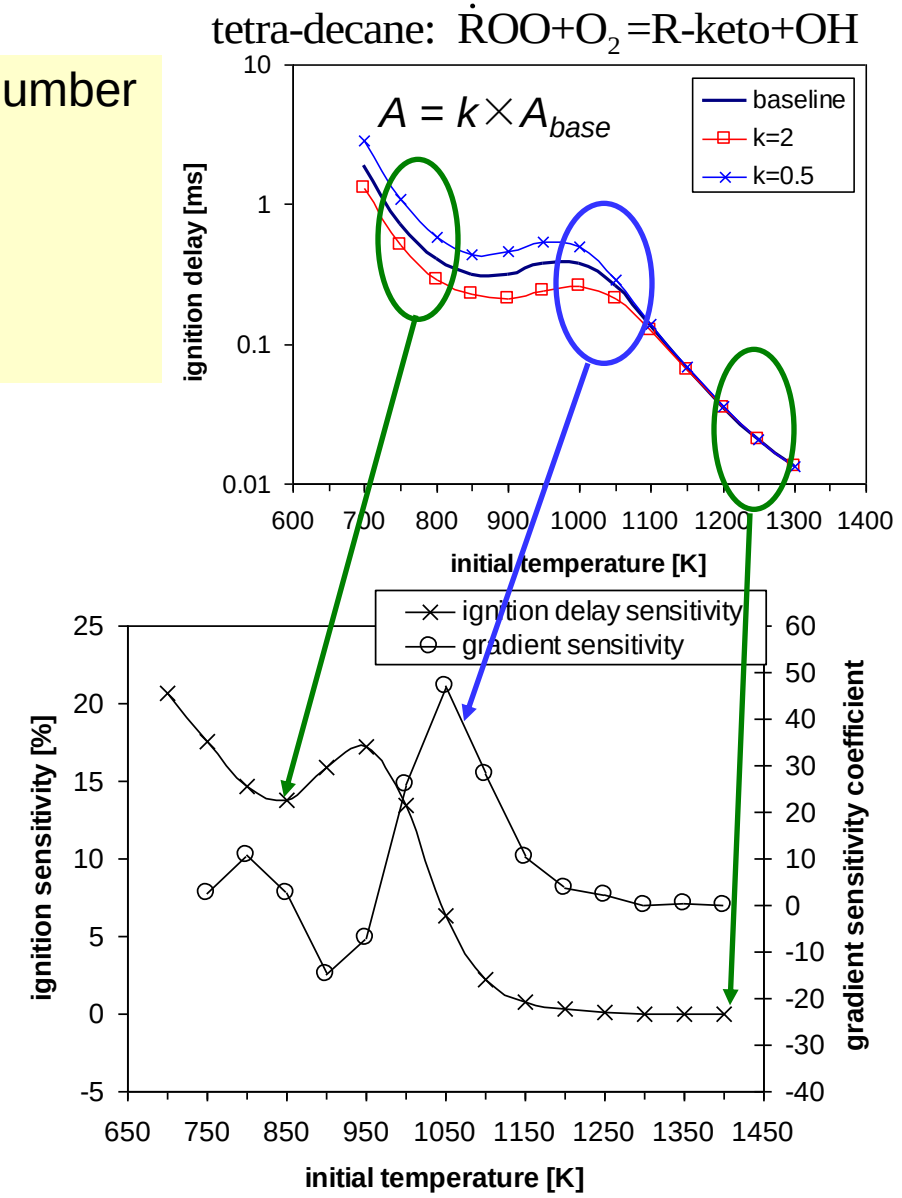
Ignition delay sensitivity coefficient

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

Ignition delay gradient sensitivity coefficient

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

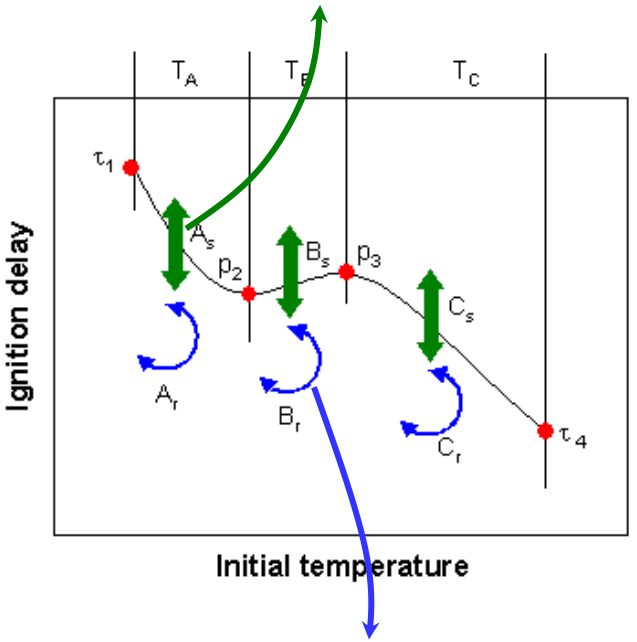
Positive S_{gr}: counter-clockwise rotation
Negative S_{gr}: clockwise rotation



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

Ignition delay sensitivity coefficient



Ignition delay gradient sensitivity coefficient

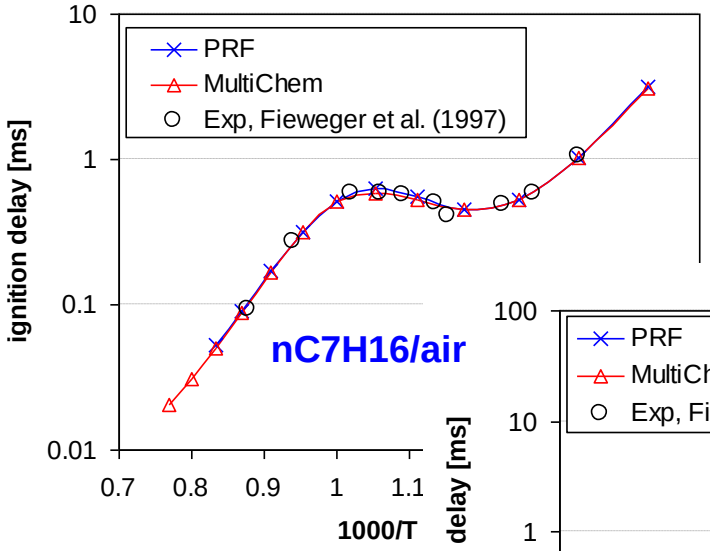
Sensitivity of ignition delay curves of n-heptane oxidation
- solid circle, open circle and blank entry denote dominant, mild and not significant influence, respectively.
- *C* indicates counter-clockwise rotation.
- Circle only indicates clockwise rotation.

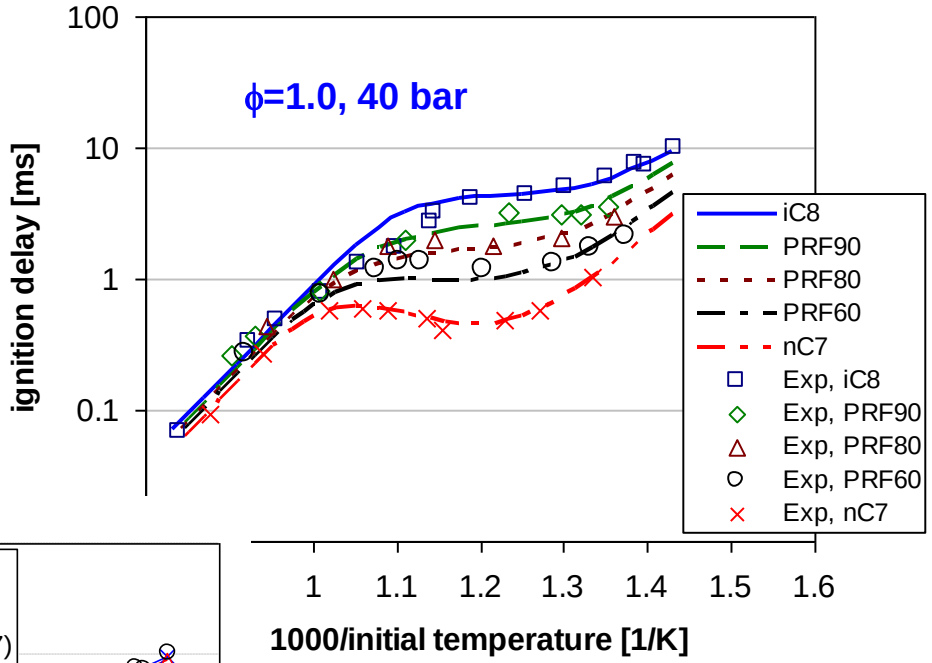
Ra, 2008

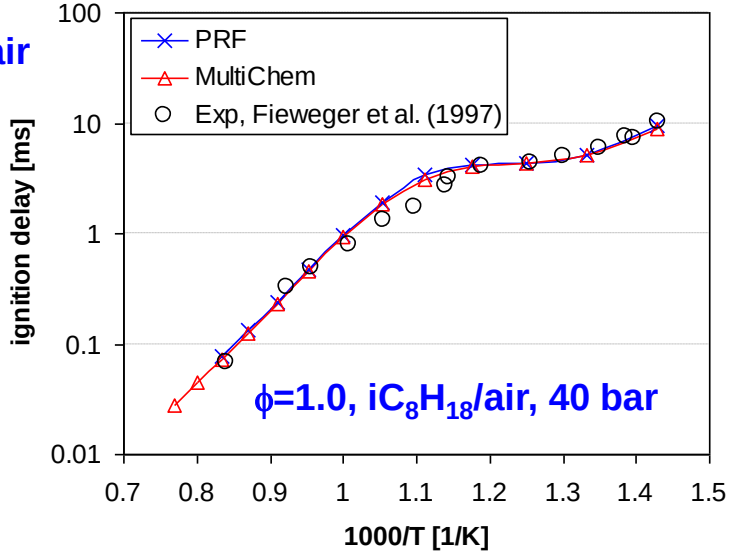
ERC-MultiChem: PRF

41 species, 158 reactions ➔ base mechanism

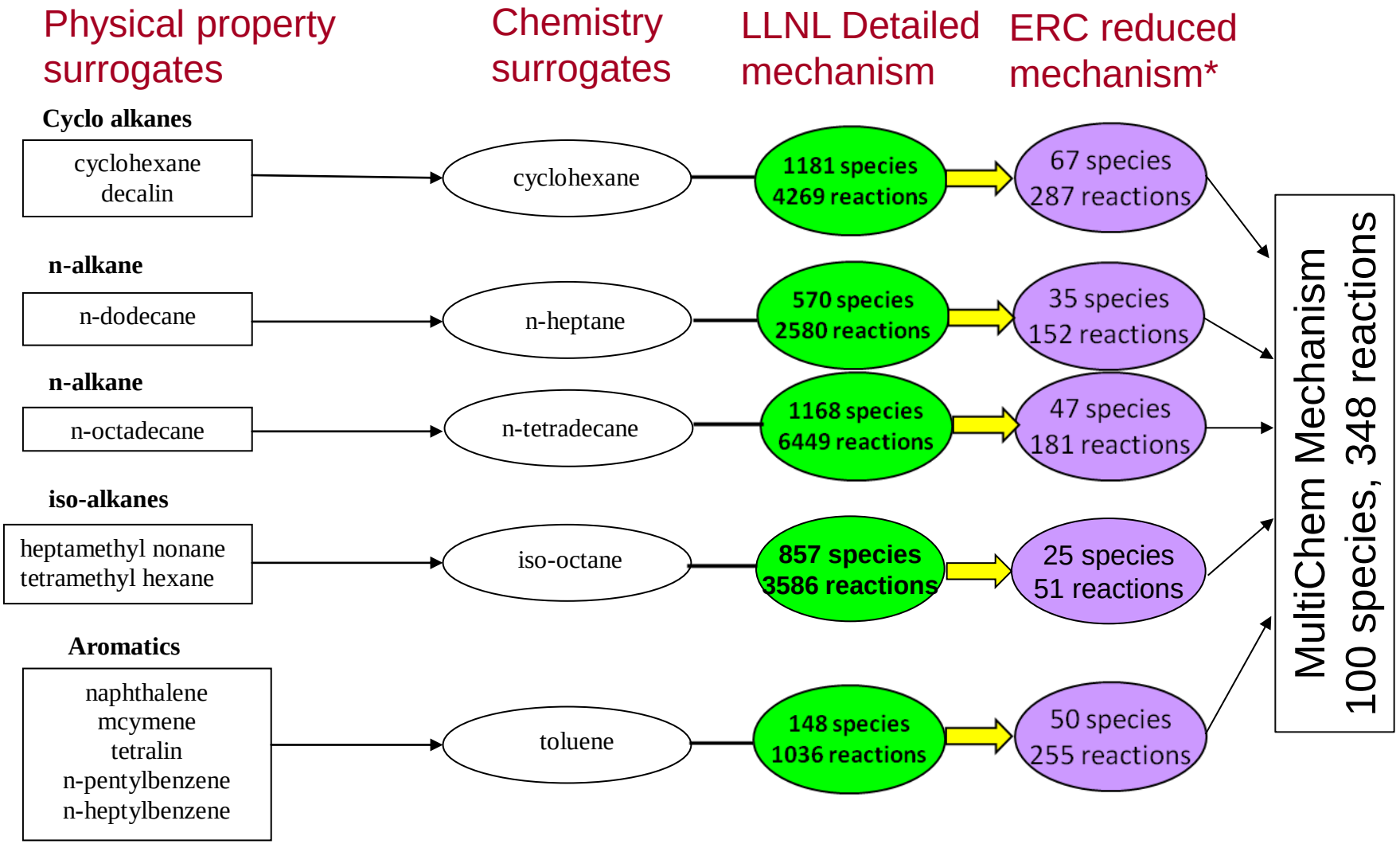
Source mechanisms: LLNL n-heptane (560 species; 2,539 reactions), isooctane (857 species; 3,606 reactions), ERC n-heptane (29 species; 52 reactions)







Chemical class grouping: "MultiChem" skeletal mechanism

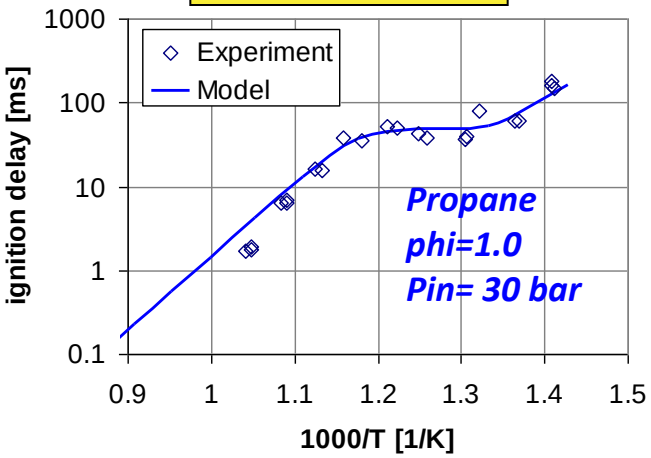


Ra, 2011

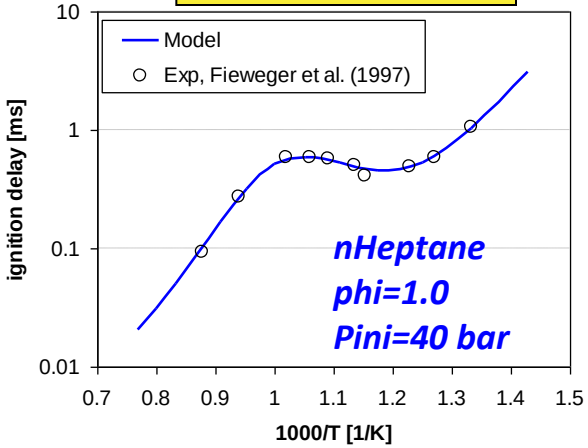
Ignition delay validations - "MultiChem"

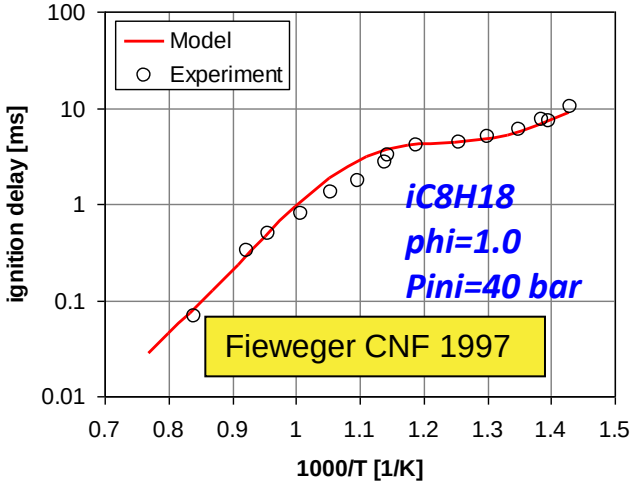
8 Surrogate fuels: *n-heptane, iso-octane, tetradecane, cyclohexane, toluene, decalin, ethanol, MB/D……*

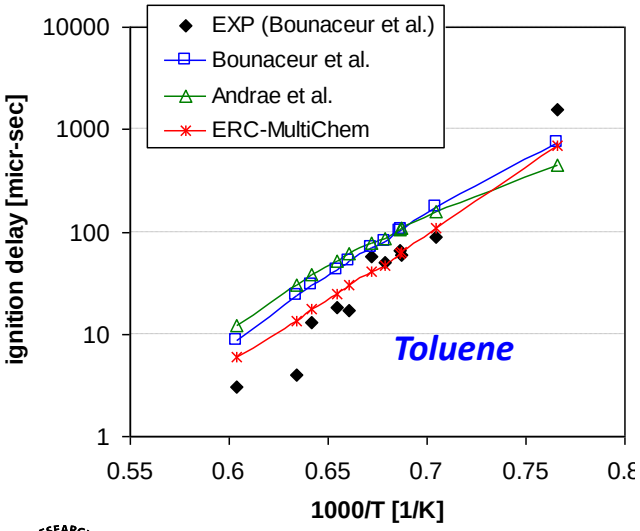
Gauthier CNF 2004

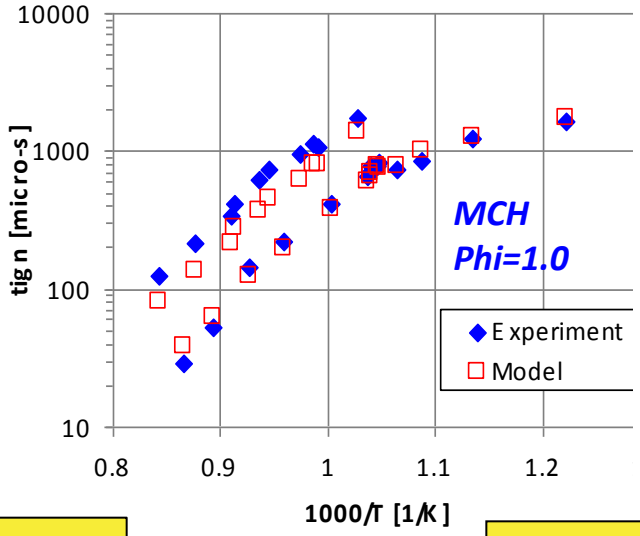


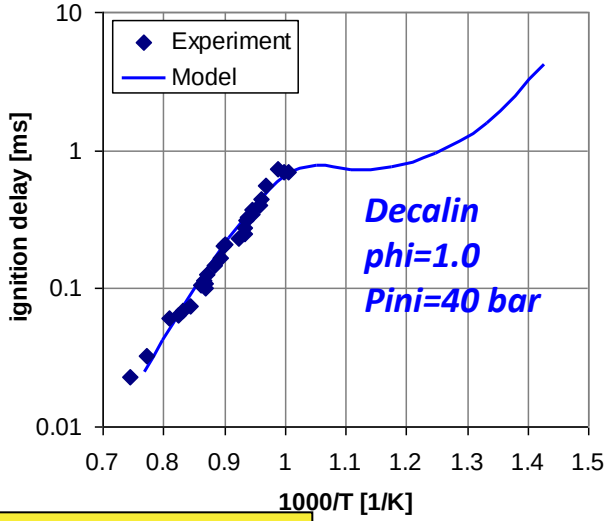
Fieweger CNF 1997











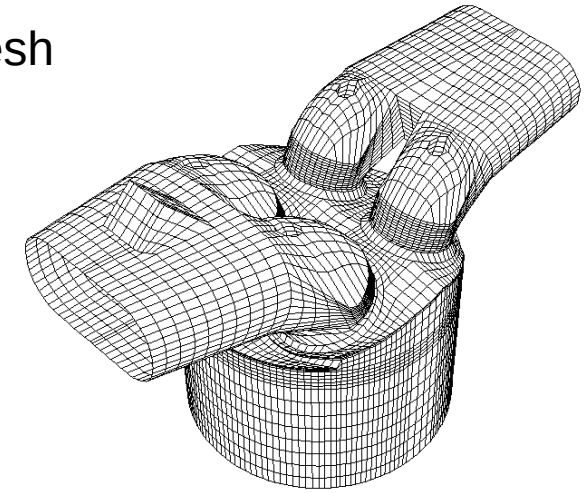
Bounaceur IJCK 2005; Andrae CNF 2005

Shen,Energy & Fuels, 2009

Amsden, 1997

3-D CFD modeling

Solve conservation equations on (moving) numerical mesh



Mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{\rho}^s$$

Species

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \cdot \left[\rho D \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s$$

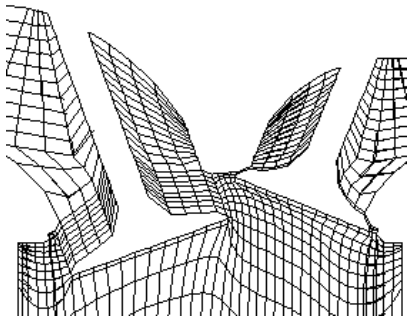
Momentum

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \rho \mathbf{g} + \mathbf{F}^s - \nabla p + \nabla \cdot \bar{\sigma}$$

combustion source terms

Energy

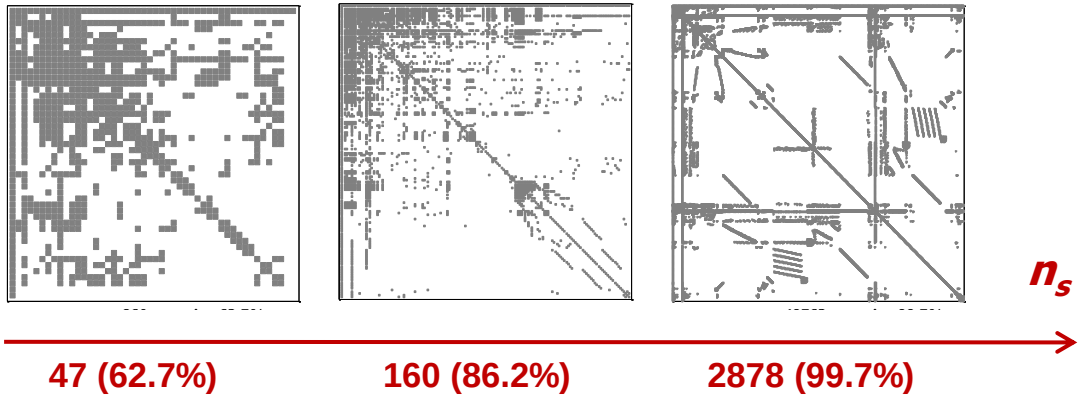
$$\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\nabla \cdot \mathbf{J} + \dot{Q}^c + \dot{Q}^s - p \nabla \cdot \mathbf{u} + \bar{\sigma} : \nabla \mathbf{u}$$



3-D CFD: Improved solver numerics

Sparse analytical Jacobian formulation

Sparsity of hydrocarbon fuel mechanisms increases with size



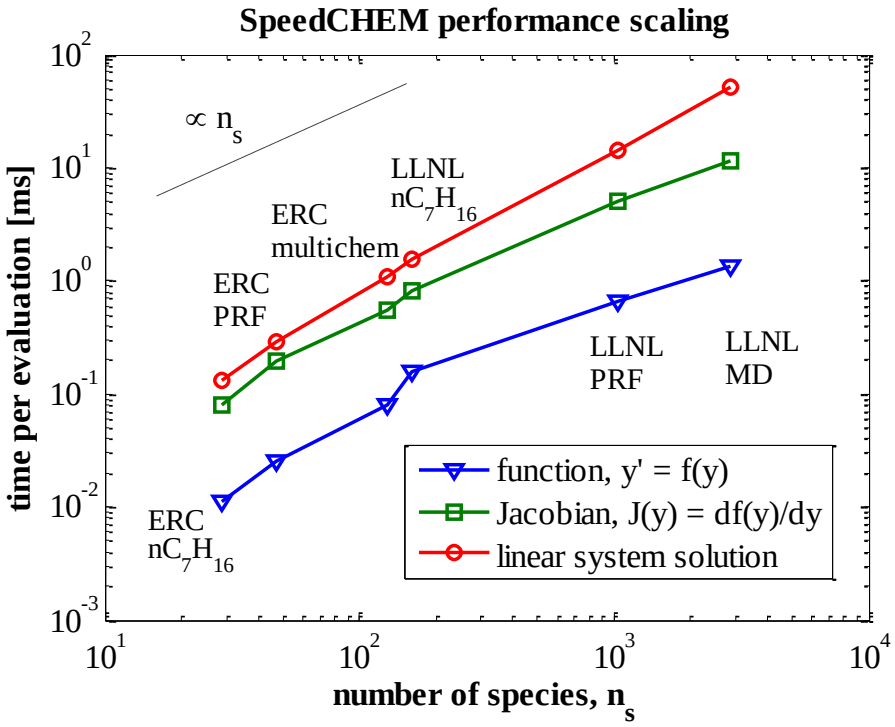
$$\frac{\partial Y^i}{\partial t} = \omega_i / \rho$$

$$\frac{\partial T}{\partial t} = -\sum_{i=1}^{n_s} \frac{\Delta h^0_{f,i} \omega_i}{\rho c_p}$$

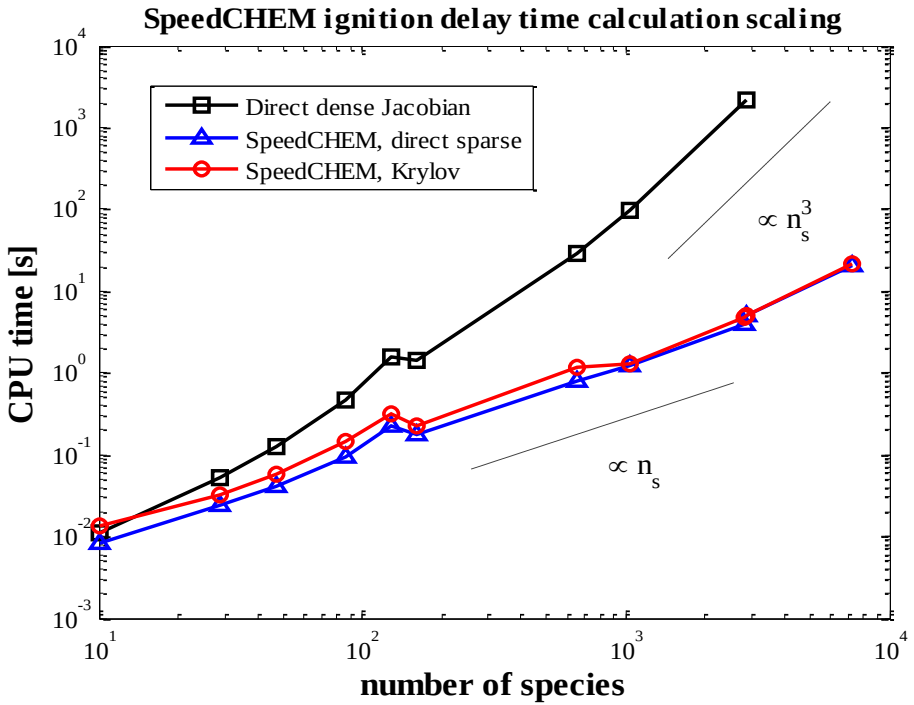
$$\mathbf{J} = \begin{array}{|cc|} \hline \textcircled{4}\ \partial\dot{T}/\partial T & \partial\dot{T}/\partial Y_j\ \textcircled{2} \\ \partial\dot{Y}_i/\partial T & \partial\dot{Y}_i/\partial Y_j \\ \textcircled{3} & \textcircled{1} \\ \hline \end{array}$$

All functions and equations are evaluated in matrix form

ODE system function, analytical Jacobian evaluation and linear system solution achieve linear scaling with n_s



3-D CFD: Improved solver numerics



9 reaction mechanisms tested

-n_s = 29 to 7171
-n_r = 52 to 31669

18 ignition delay calculations per mech

- phi = [0.5, 1.0, 2.0]
- T_0 = [650, 800, 1000] K
- p_0 = [20, 50] bar
- t = [0.1] s

Promising, efficient approach for **practical engine simulations**

1. Numerically exact solution (no mechanism reduction or manipulation).
2. Speed-up of more than three orders of magnitude at large sizes (n_s>1000)
3. Even for modest sizes (~50-500 species), overall CPU time for chemistry is reduced by 3-10 times in comparison with dense chemistry integrators
4. Preconditioned Krylov solution for future, very large mechanisms

Liang, 2009
Shi, 2012
Perini, 2014

Efficient chemistry solvers – cell clustering

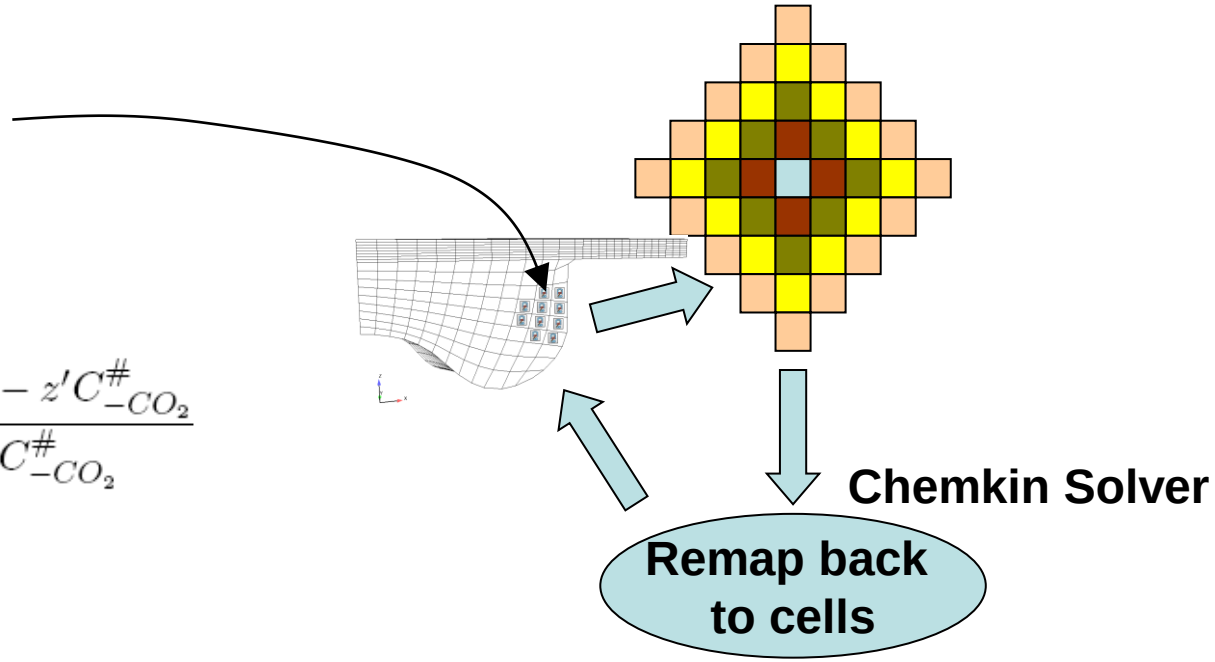
Group thermodynamically-similar cells to reduce the calling frequency to save computer time - Adaptive Mechanism Clustering (AMC) scheme

Extended dynamic adaptive chemistry (EDAC) scheme

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)

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

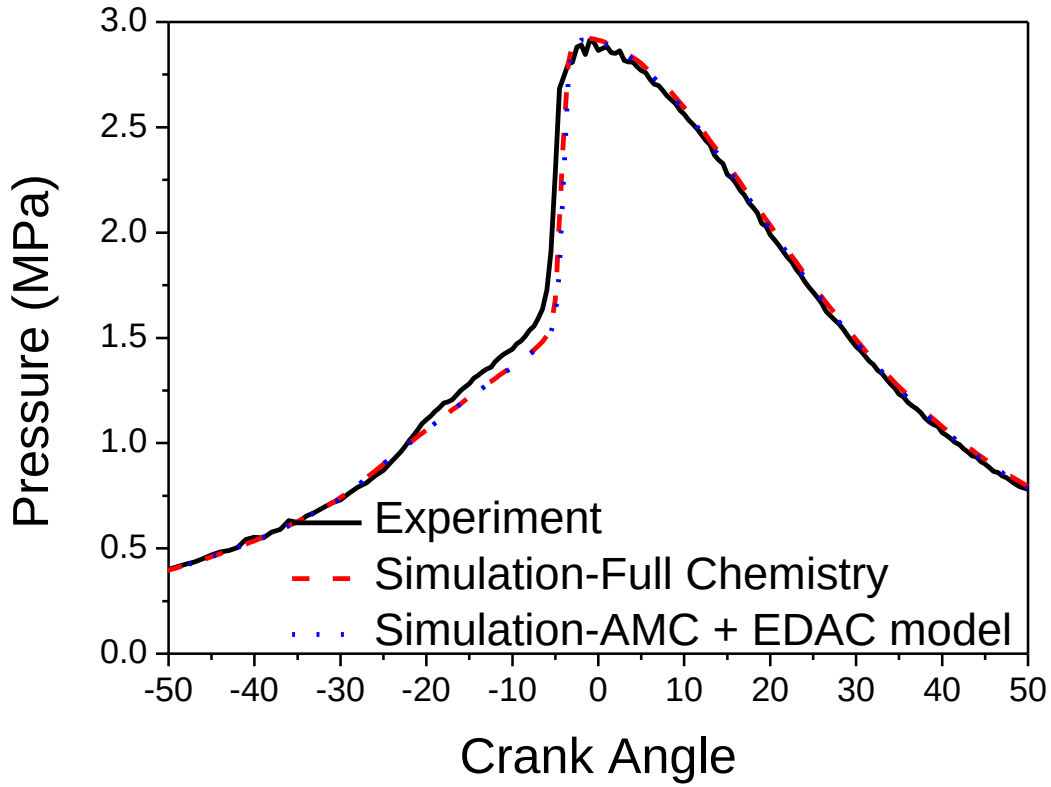


Shi, 2012

HCCI engine validation

ERC PRF mech.
(39 sp, 141 rxn)

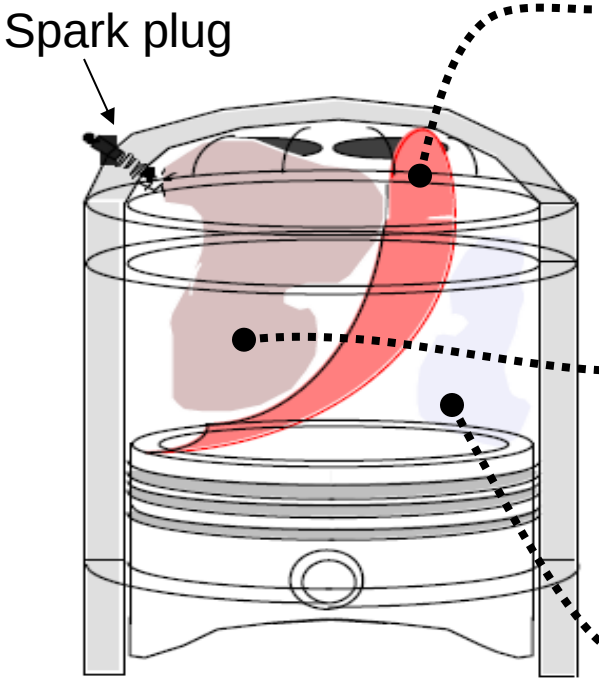
Full	AMC	AMC+EDAC
48.27 hrs.	3.99 hrs.	2.88 hrs.



Liang, 2006

SI engine combustion modeling

Flame propagation Models with Detailed Chemistry



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

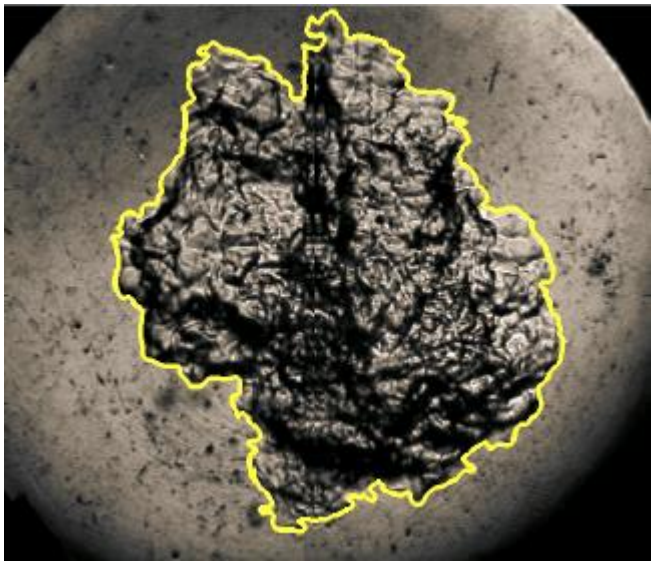
Post-flame Chemistry

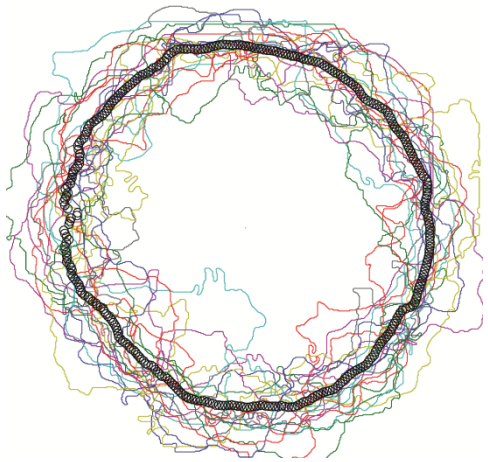
- CO oxidation, H_2-O_2 reactions
- Pollutant formation mechanisms

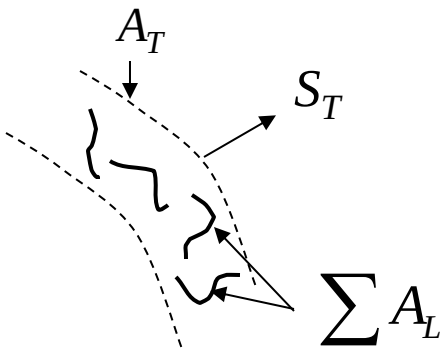
Knocking Combustion

- Auto-ignition mechanisms
- Location / intensity

What is a turbulent flame?







Ensemble of thin (laminar) flamelets, interacting with the flow turbulence.

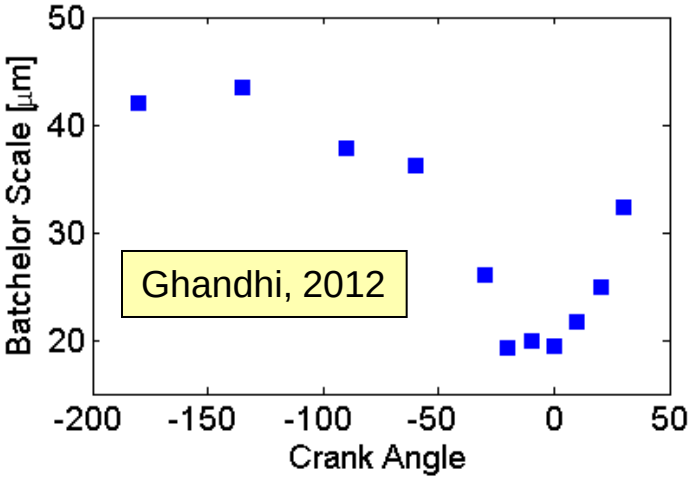
Due to increased surface area, turbulent flame "brush" propagates at enhanced velocity

$$S_T = S_L \frac{\sum A_L}{A_T}$$

Turbulent flame structure

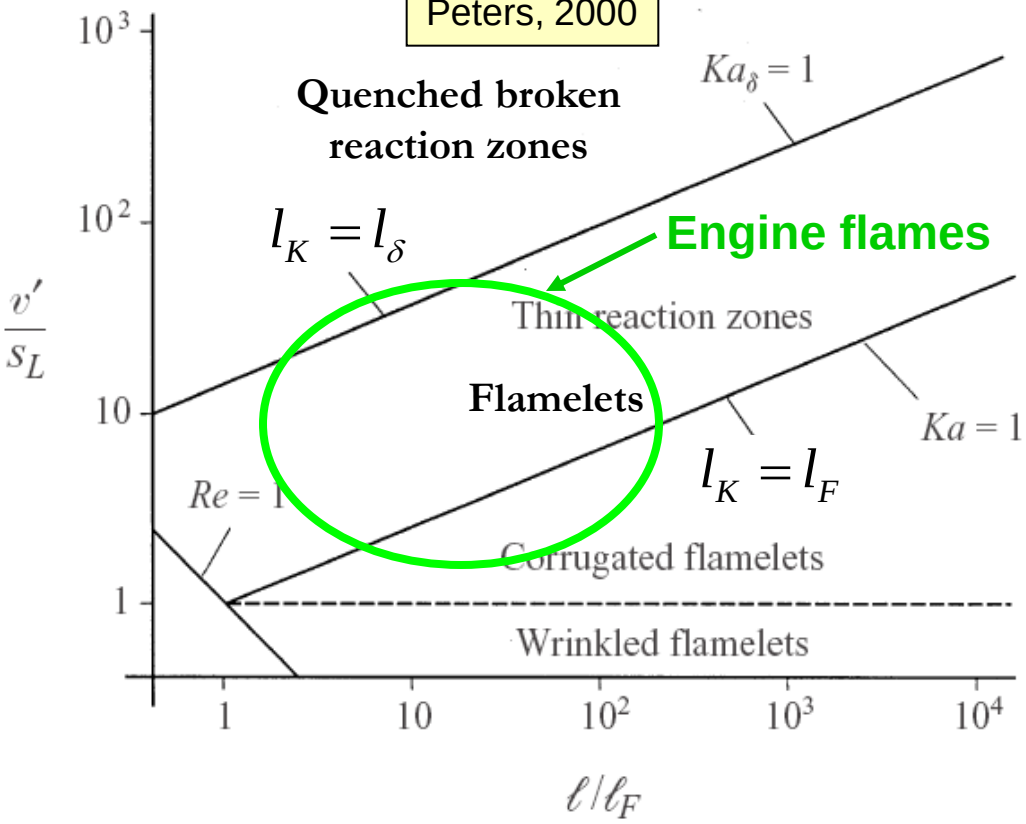
Kolmogorov/Batchelor length scales:

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



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, 2007

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

Reitz, 1981

Laminar flame speed: balance between reaction and diffusion

$$\left.\begin{aligned}\frac{\partial Y_i}{\partial t} &= D\frac{\partial^2 Y_i}{\partial x^2} + \omega_i/\rho \\ \frac{\partial T}{\partial t} &= D\frac{\partial^2 T}{\partial x^2} - \sum_{i=1}^{N}\Delta h^0_{f,i}\omega_i/\rho c_p\end{aligned}\right\} \quad S_T = \sqrt{D_T\frac{d\tilde{Y}_i}{dt}}$$

- Mallard, Le Chatelier

Consider the single component system:

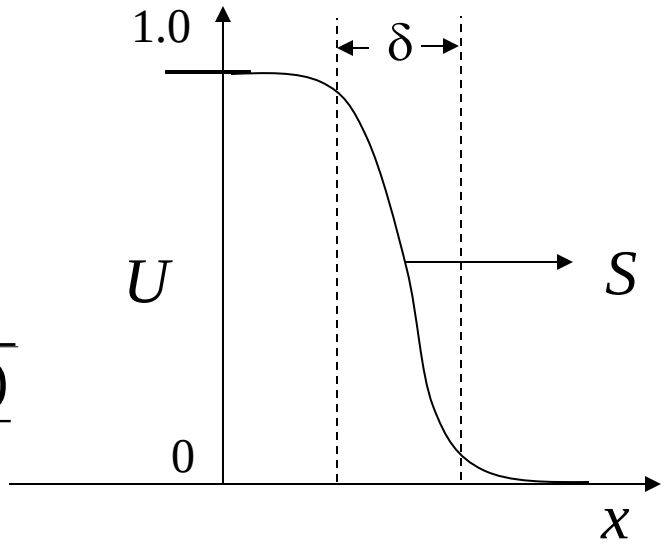
$$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2} + F(U) \quad \text{with } U = \frac{T - T_{unburned}}{T_{burned} - T_{unburned}} \quad \text{and} \quad F(U) = \beta U^{m+1}(1-U)^m$$

Admits a traveling wave solution

$$U(x - St) = [1/(1 + e^{\frac{mS}{D}(x-St)})]^{1/m}$$

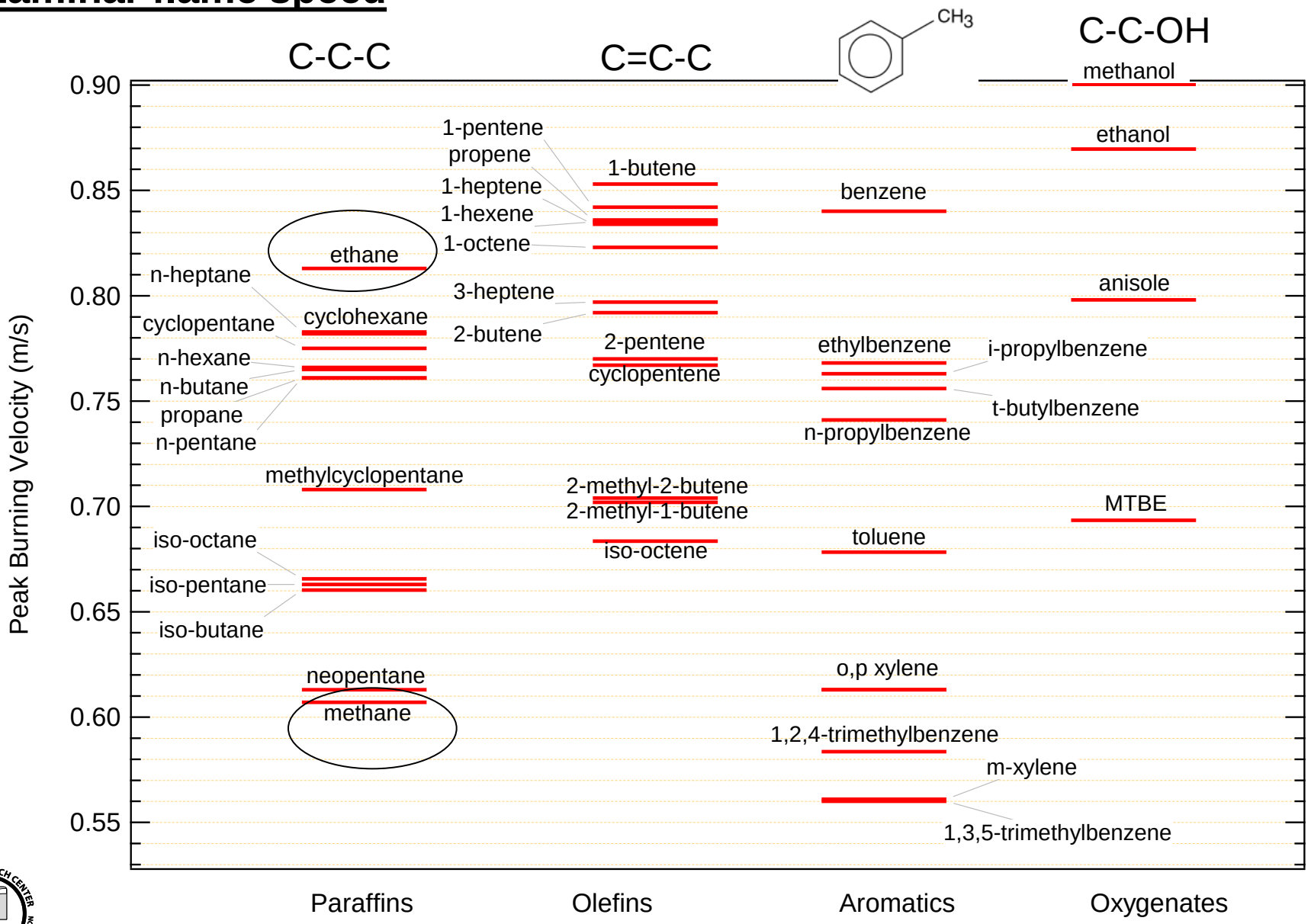
where

$$S = \sqrt{\frac{D\beta}{m+1}} \quad \text{and} \quad \delta = \frac{D}{mS} = \sqrt{\frac{D(m+1)}{\beta m^2}}$$



Farrell, 2005

Laminar flame speed

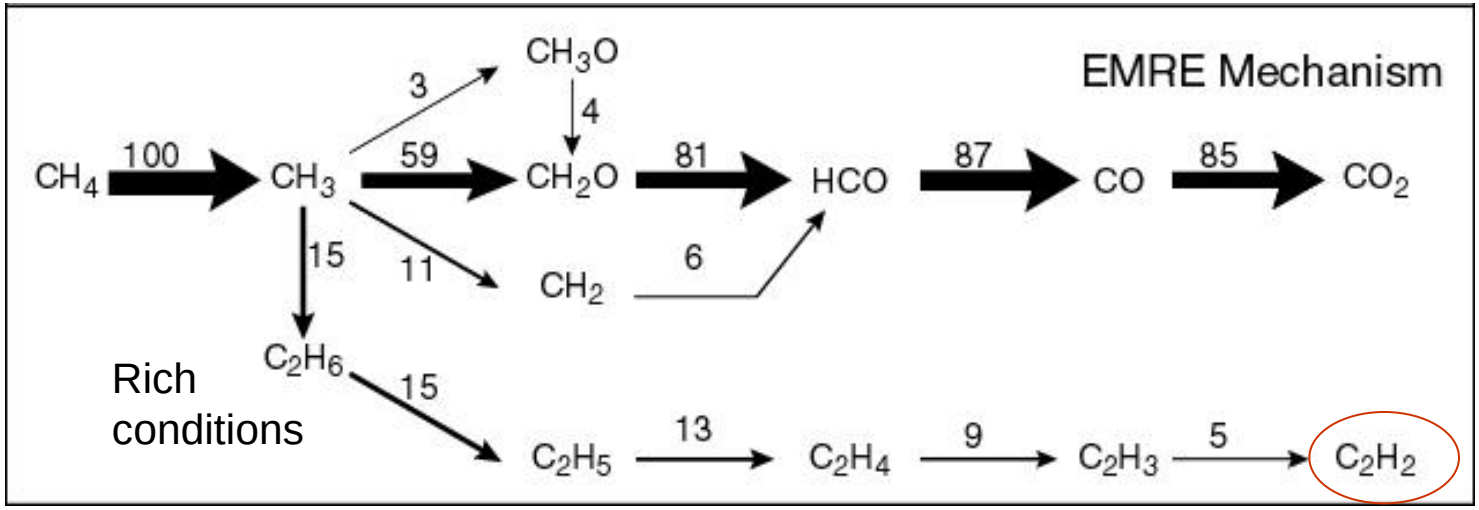


Lutz, 1988

Importance of chemistry - Methane

Flux analysis: oxidation proceeds through methyl

– slow path, high activation energy due to tight C-H_3 bonds



Acetylene

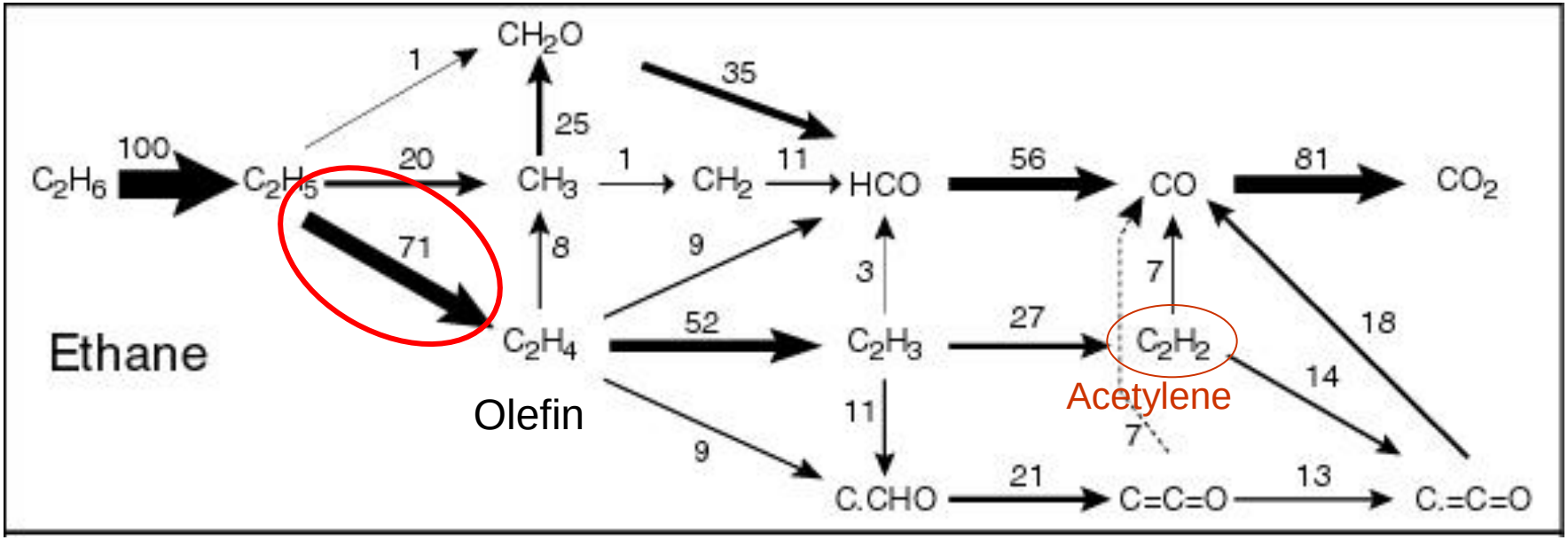
Lutz, 1988

Importance of chemistry - Ethane

- Limited flux through slow methyl channels
  - hydrogen abstraction leaves weaker secondary C-H_2 bonds
- Greater flux through chain branching pathways, e.g.,

$$H + O_2 \leftrightarrow OH + O$$

- Ignition delays are very sensitive to rates of H atom production

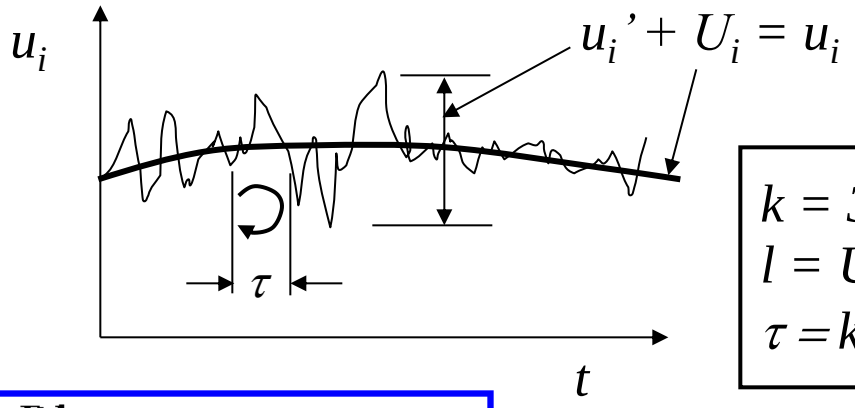


Ignition delay Ethane < Ignition delay Methane

Wang, 2012

Diffusion: Turbulence models

(RANS - RNG k-ε)



$$k = 3u_i^2/2$$
$$l = U_i\,\tau$$
$$\tau = k/\varepsilon$$

$$\rho\frac{Dk}{Dt} = P - \rho\varepsilon + Diffusion$$

$$\rho\frac{D\varepsilon}{Dt} = C_1\frac{P\varepsilon}{k} - C_2\rho\frac{\varepsilon^2}{k} + Diffusion - R + C_3\rho\varepsilon(\nabla\cdot\mathbf{u})$$

$$R = \frac{C_\mu\rho\eta^3(1-\eta/\eta_0)}{1+\beta\eta^3}\frac{\varepsilon^2}{k}$$

$$\eta = \frac{k}{\varepsilon}\sqrt{2S_{ij}S_{ij}}$$ ~ turbulent/mean flow time scale

$$D_T = C_\mu k^2/\varepsilon$$

Production

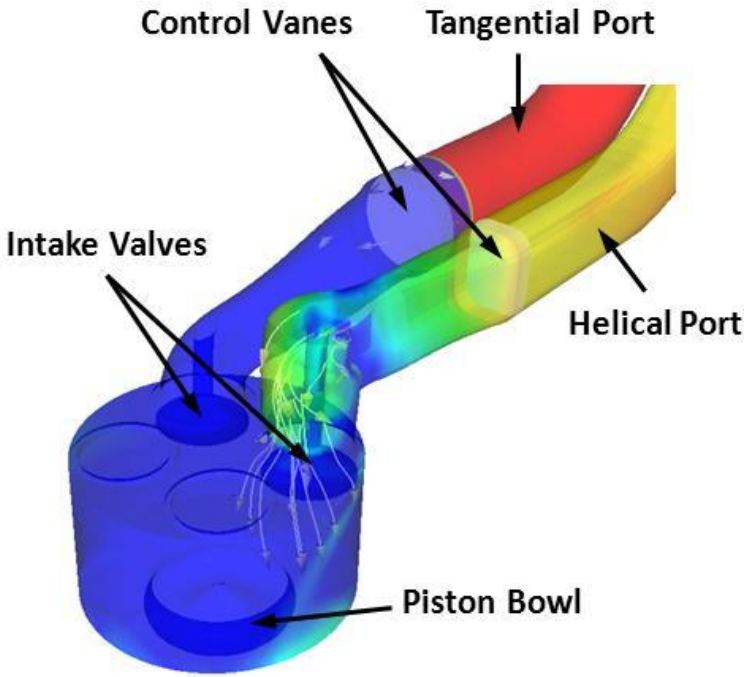
$$P = -\rho u_i u_j S_{ij}$$

Mean flow strain rate

$$S_{ij} = \frac{1}{2}(\partial u_i/(\partial x_j + \partial u_j/\partial x_i)$$

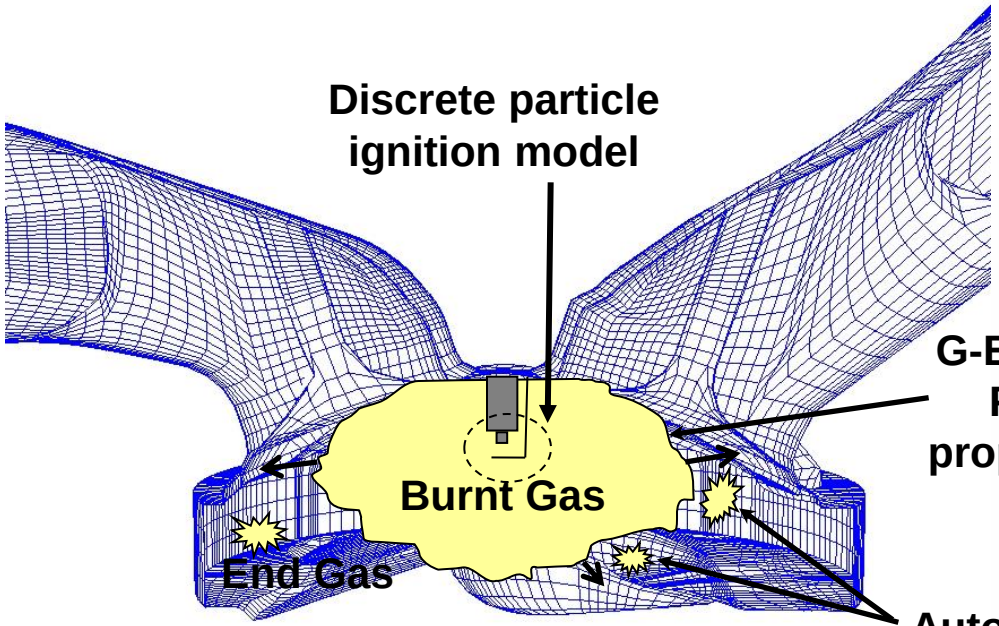
Reynolds stresses

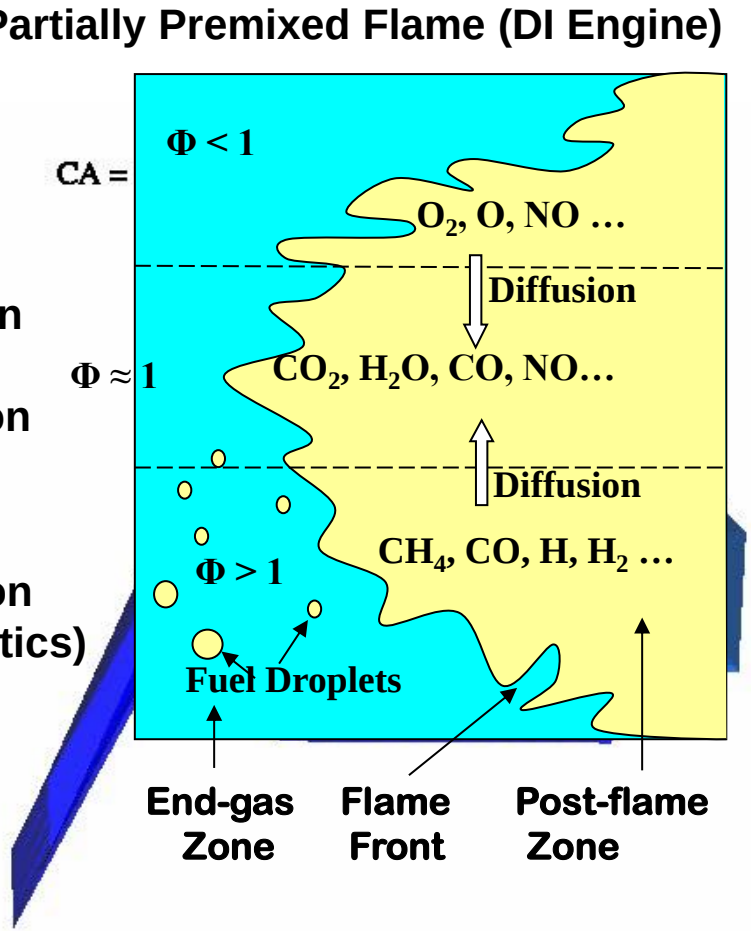
$$u_i u_j - \frac{2}{3}k\delta_{ij} = -2v_t(S_{ij} - \frac{1}{3}(\nabla\cdot u)\delta_{ij}$$



Liang, 2007

Ignition and level set (G-equation) models





S_T from flame speed correlations

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

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

Liang, 2007

Turbulent flame speed correlations

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

Peters, 2000

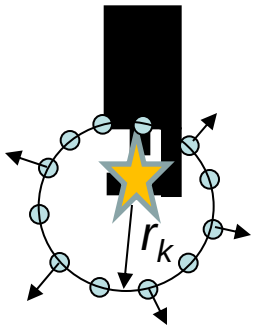
Stretch factor:

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

Discrete Particle Ignition Kernel (DPIK) model

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

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



Fan, 2000

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

Liang, 2007

Laminar flame speed correlations

Power Law (Metghalchi & Keck, 1982):

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

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

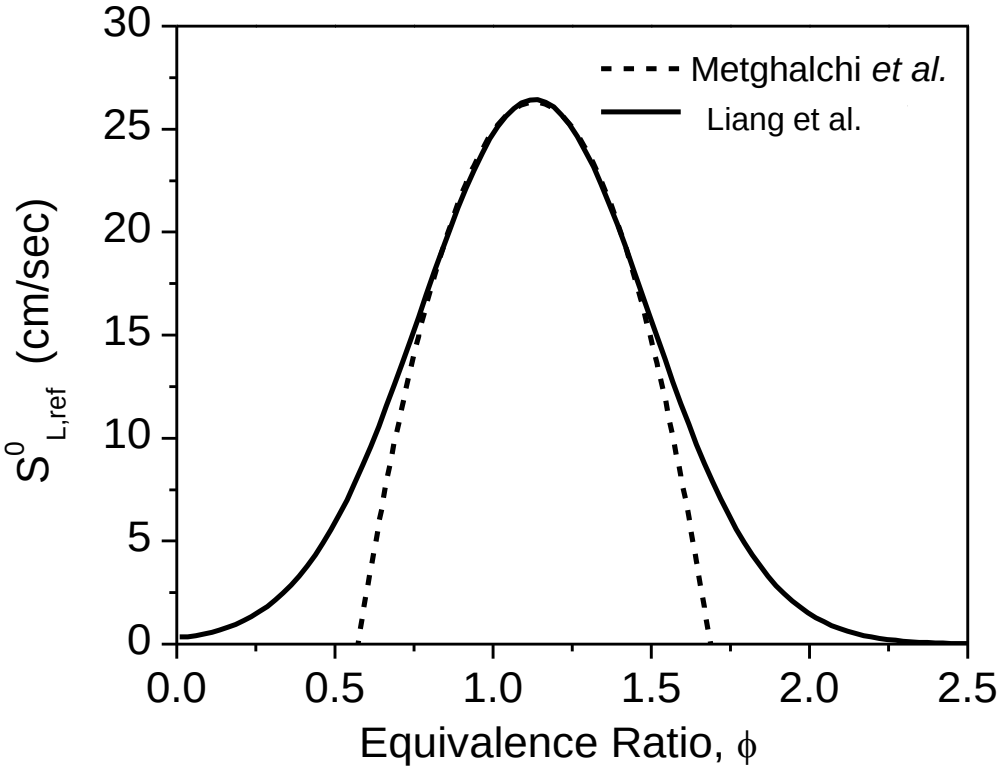
$$\beta = -0.16 + 0.22(\varphi - 1)$$

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, $\omega = 26.9$ $\eta = -0.134$ $\xi = 3.86$ $\sigma = 1.146$

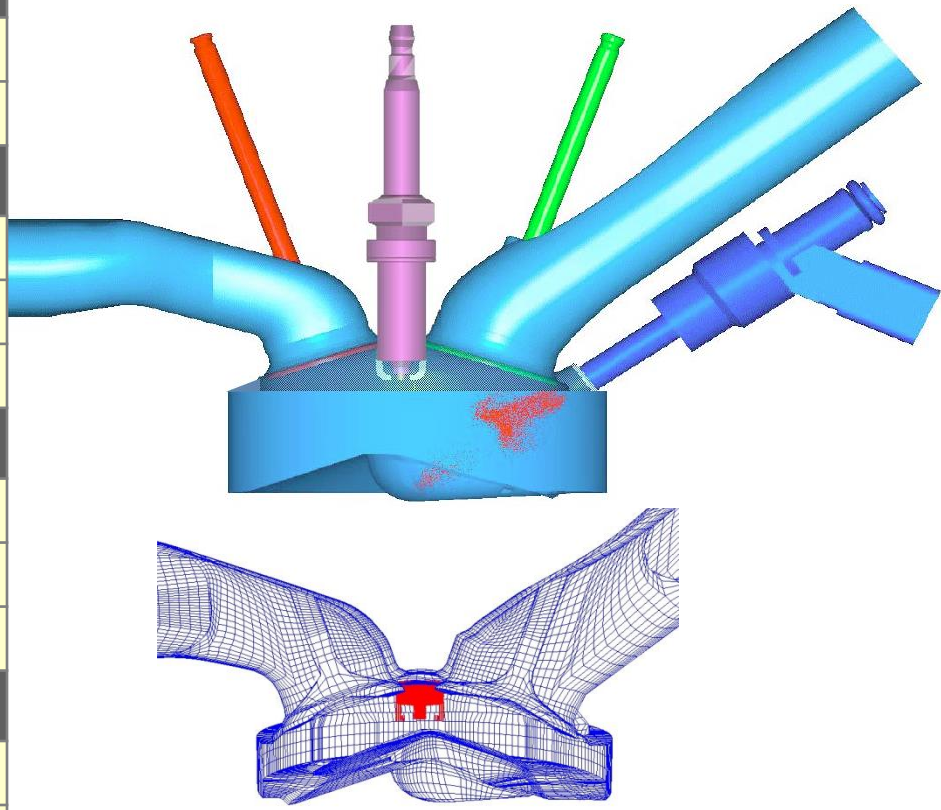
Liang, 2007

Validation - PFI/DI gasoline engines

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

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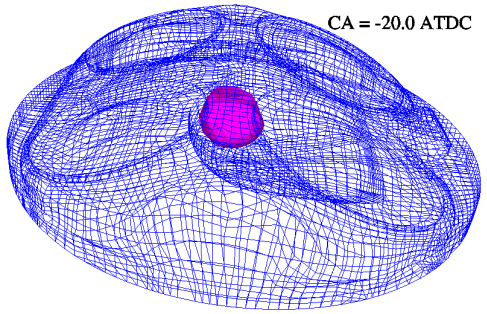
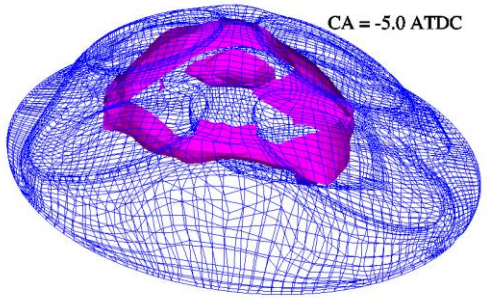
Validation - PFI engine operation

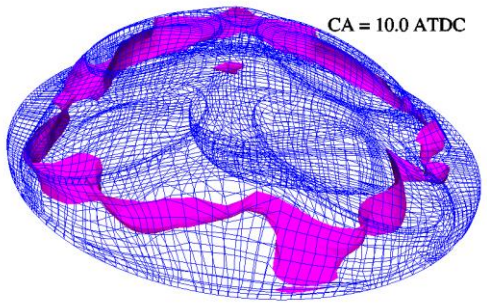
Spark Timing = 40 BTDC



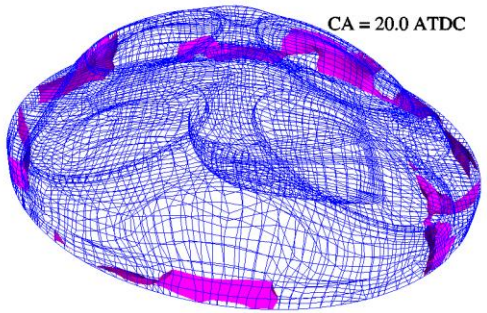
CA = -20 ATDC



CA = -5 ATDC

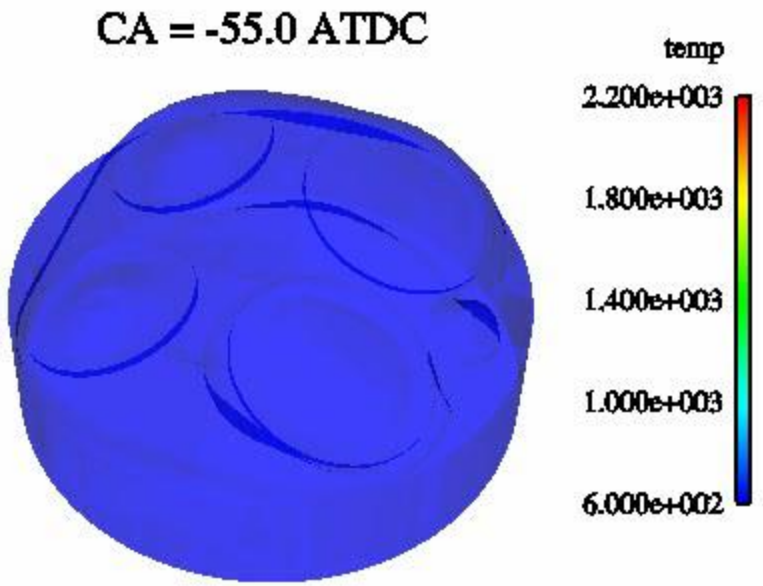


CA = 10 ATDC



CA = 20 ATDC

Evolution of the *G*=0 surface



Evolution of Temperature

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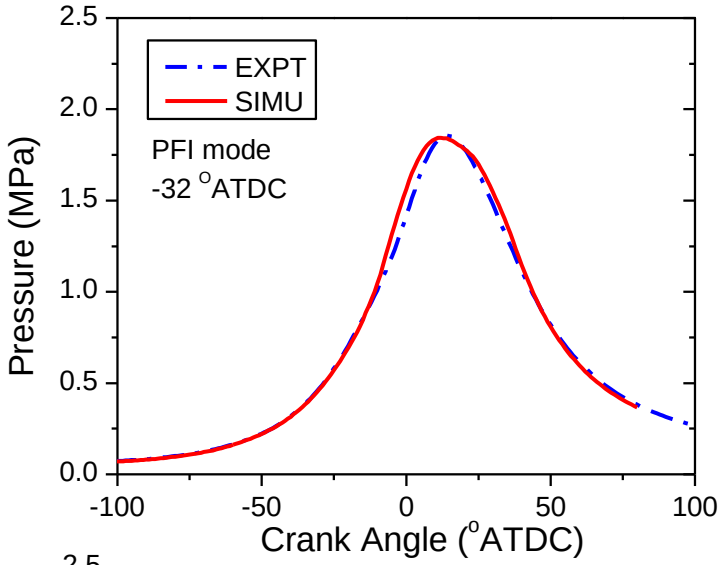
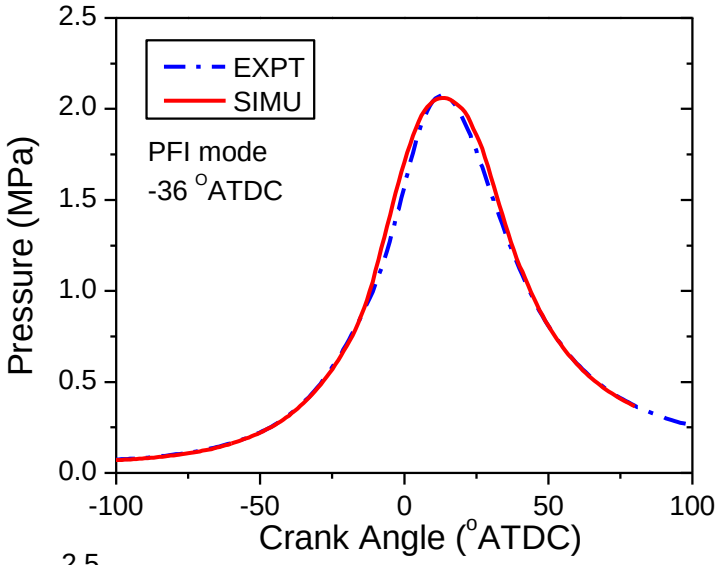
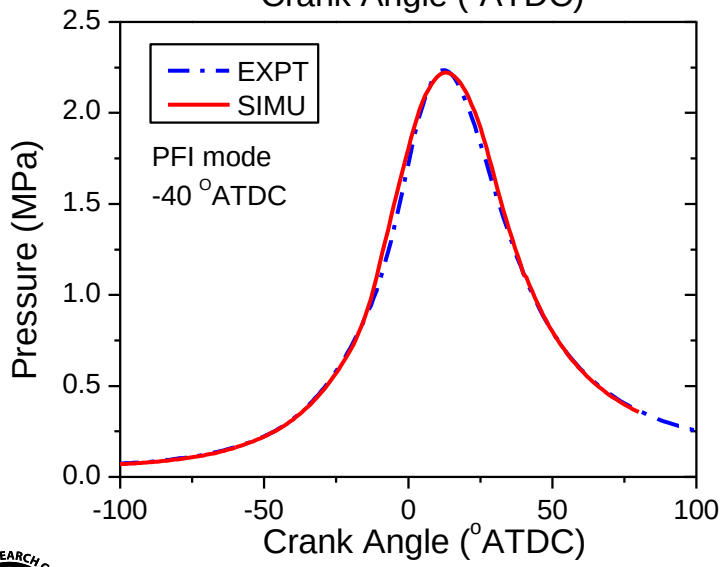
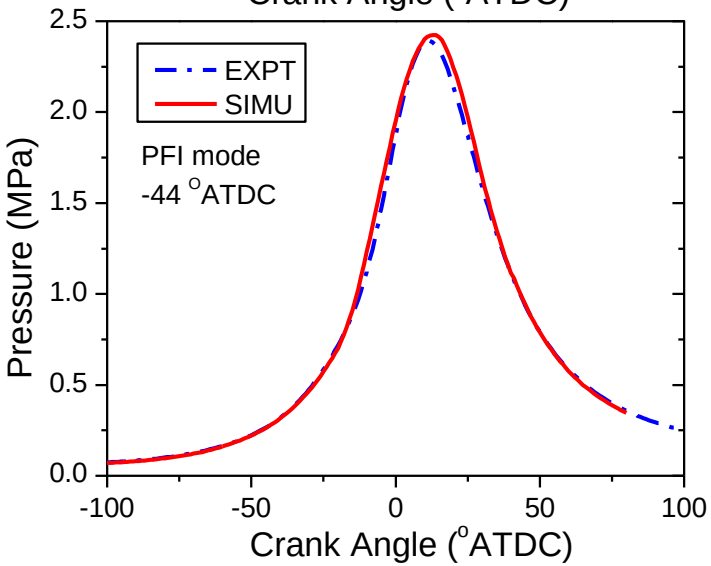
Validation - PFI engine operation









Spark Timing
-44, -40, -36, -32 ATDC
Engine Speed
1500 rev/min

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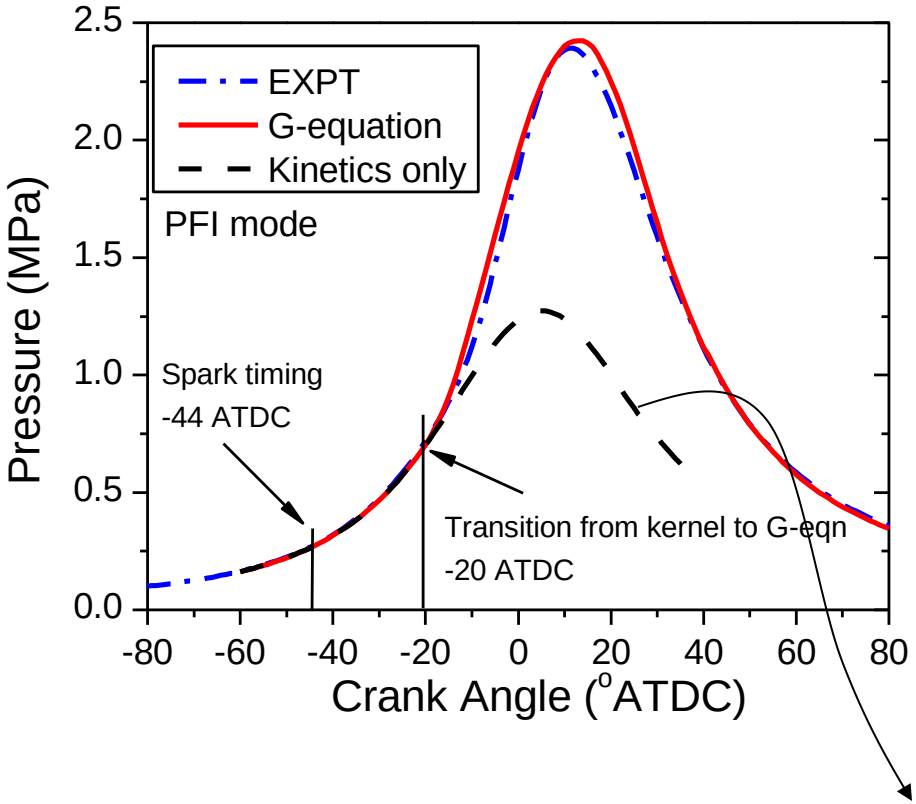
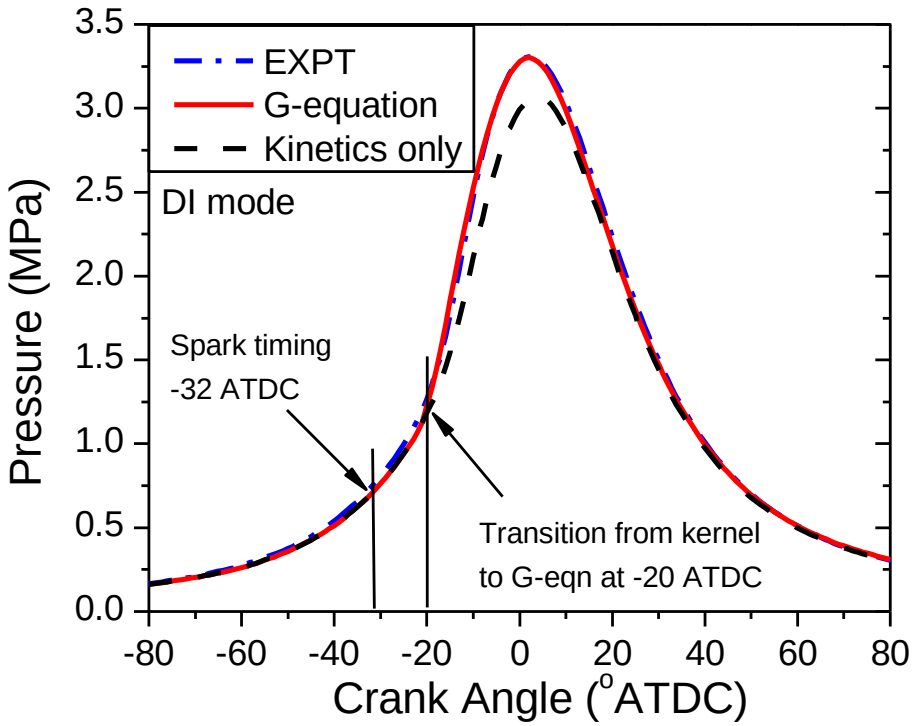
Role of flame propagation

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: $S_T = \sqrt{D\frac{dY_i}{dt}}$

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Role of flame propagation

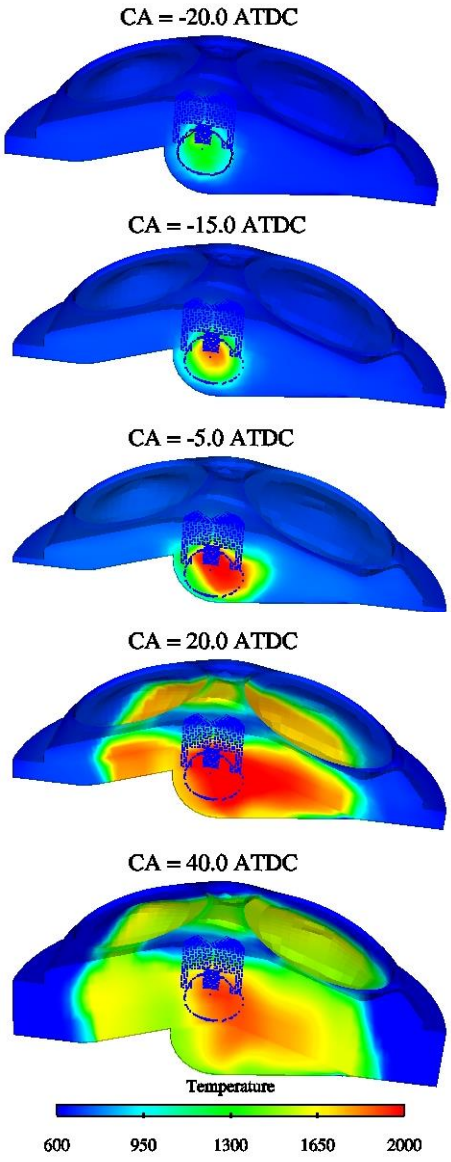
PFI case
Spark timing = -44 ATDC

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.

Kinetics Controlled



***G*-equation**