Internal Combustion Engines
I: Fundamentals and Performance Metrics

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2018 Princeton-Combustion Institute
Summer School on Combustion
Course Length: 9 hrs

(Mon.- Wed., June 25-27)

Short course outline:

Internal Combustion (IC) 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, Thermodynamics and 0-D modeling
- Hour 2: 1-D modeling, Charge Preparation
- Hour 3: Engine Performance Metrics, 3-D flow modeling

Day 2 (Computer modeling/engine processes)

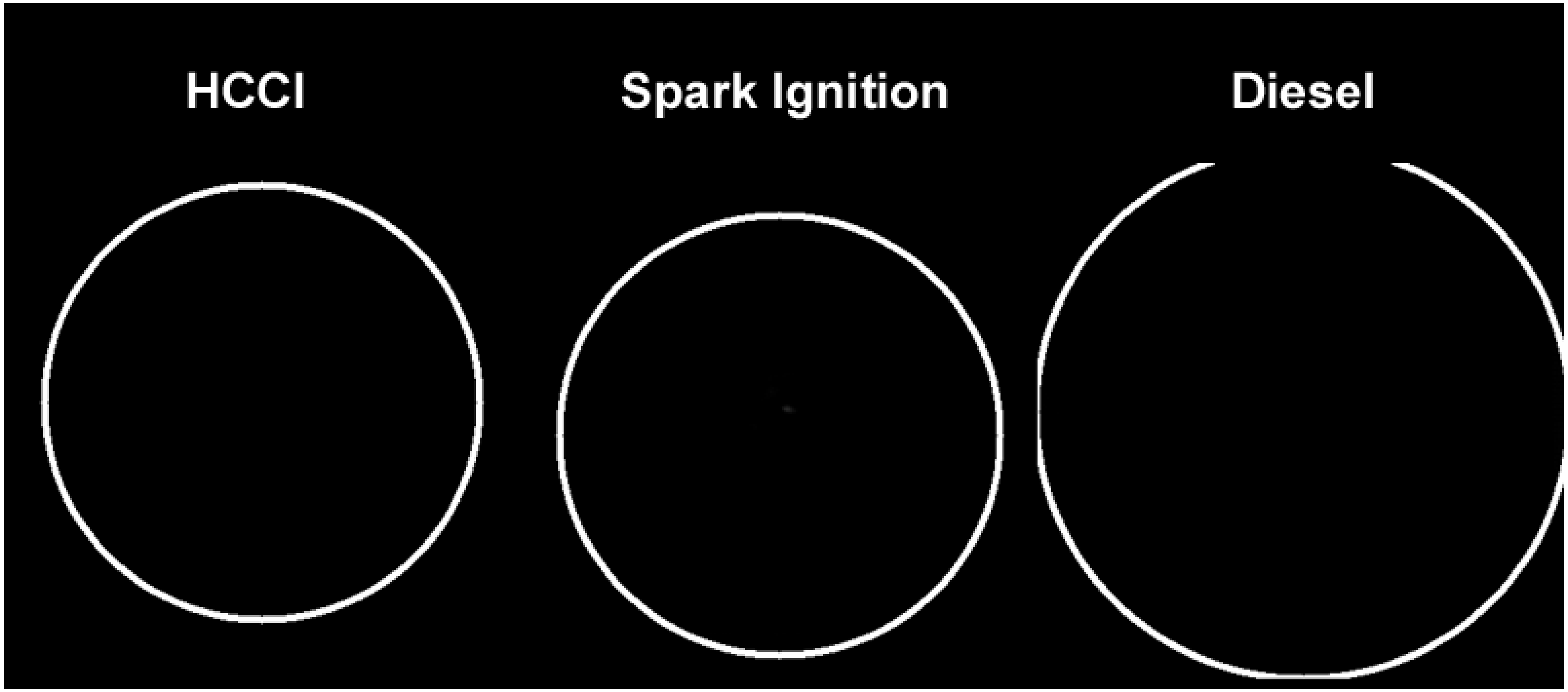
- Hour 4: Engine combustion physics and chemistry
- Hour 5: Premixed Charge Spark-ignited engines
- Hour 6: Spray modeling

Day 3 (Engine Applications and Optimization)

- Hour 7: Heat transfer and Spray Combustion Research
- Hour 8: Diesel Combustion modeling
- Hour 9: Optimization and Low Temperature Combustion

Modes of engine combustion

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



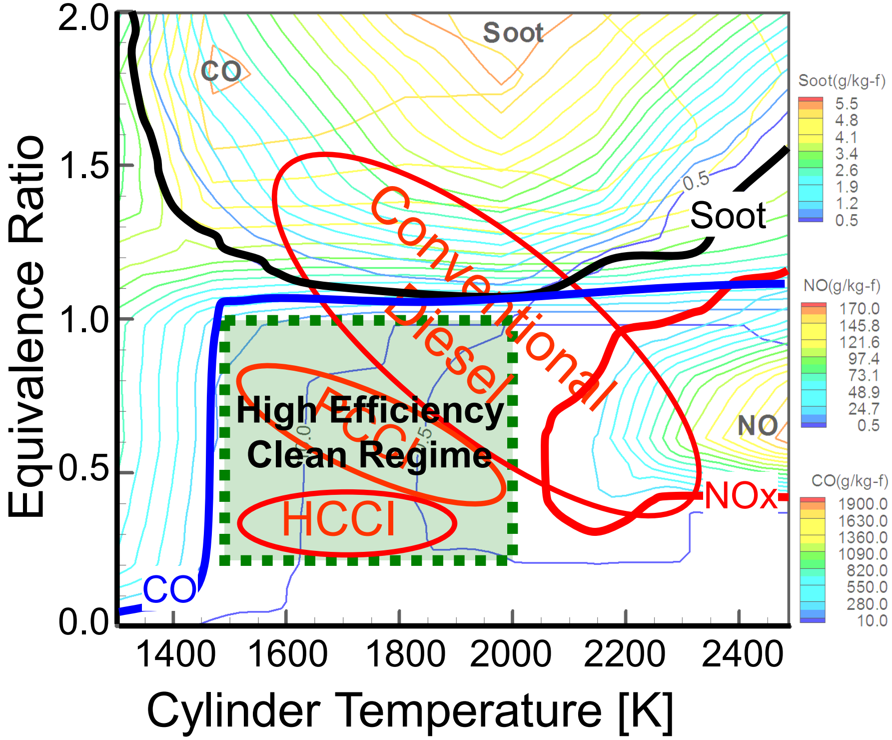
HCCI uses a hybrid combustion strategy. Premixed fuel and air is inducted, but instead of igniting with a spark as in a SI engine, the high temperature from compression causes the mixture to spontaneously react, like in a diesel engine. Ignition occurs at slightly different times at different locations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

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

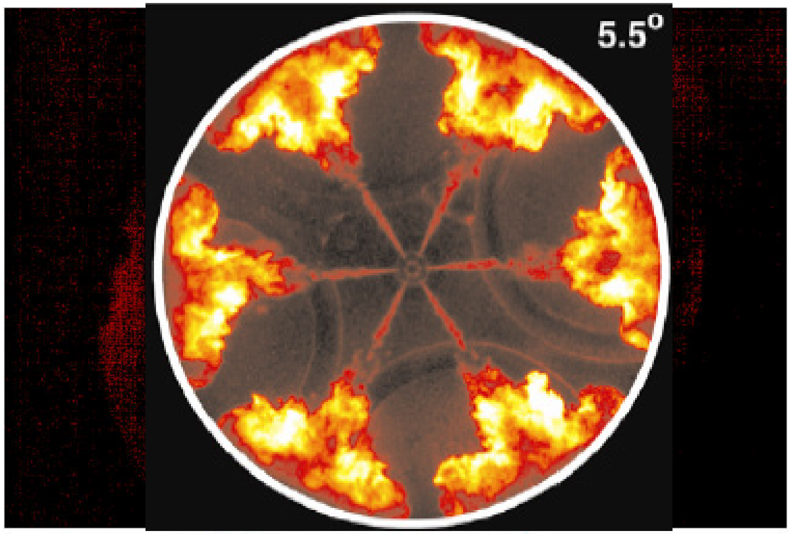
Park, 2007

IC Engine combustion regimes

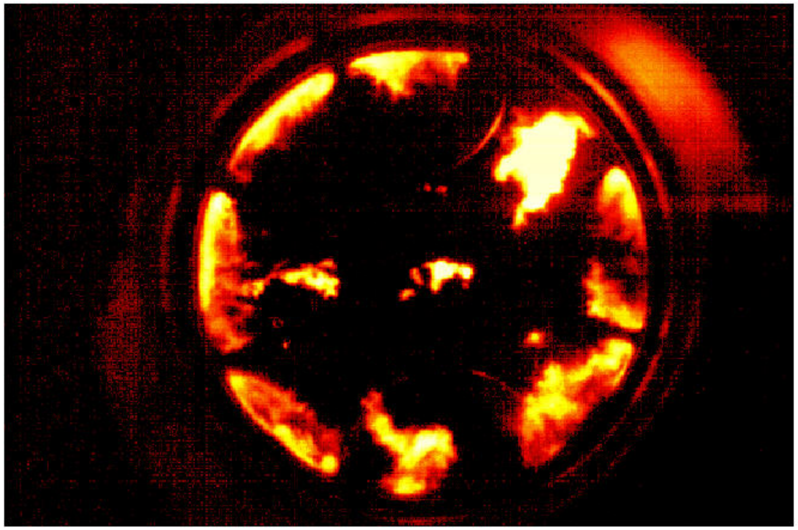
Kamimoto plot



Conventional diesel



Early injection PCCI

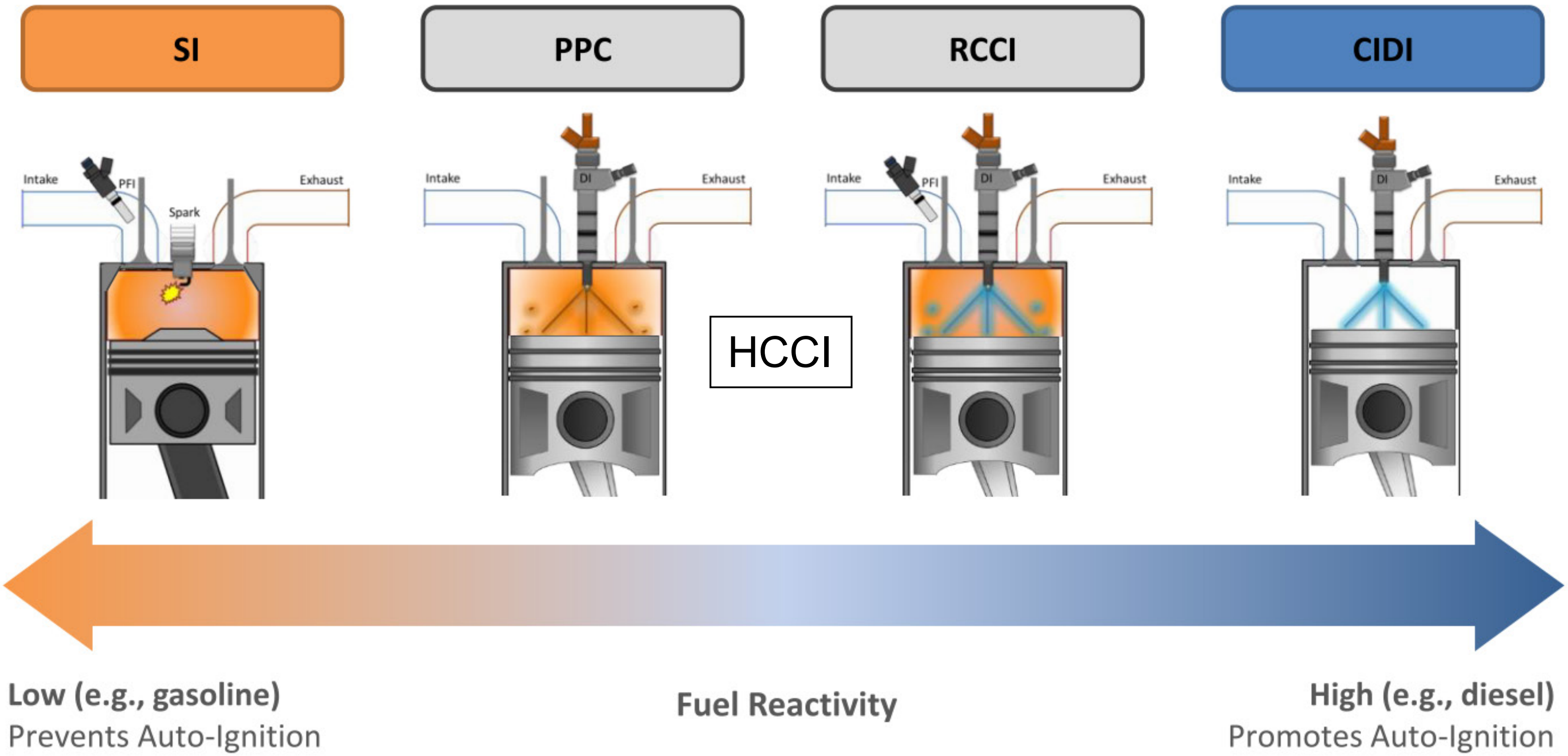


PCCI – Premixed Charge Compression Ignition

HCCI – Homogeneous Charge Compression Ignition

Daw, 2013

Advanced combustion regimes



SI – Spark Ignition (Homogeneous Charge)
PPC – Partially Premixed Charge
RCCI – Reactivity Controlled Compression Ignition
CIDI – Compression Ignition, Direct Injection

Lessons from history (1910-20) – "the Mayflower"

Ignitability affects engine operating regime - limits compression ratio (CR).

Early Spark Ignition (SI) engines were plagued by "spark knock", CR ~ 4:1.

Cylinder pressure measurements by Midgley and Kettering at DELCO/GM showed different fuels had different knock tendency

e.g., kerosene worse than gasoline

Volatility differences were thought to be the explanation.

Guided by the "Mayflower," they added a red dye (iodine) to kerosene and knock tendency was greatly reduced!

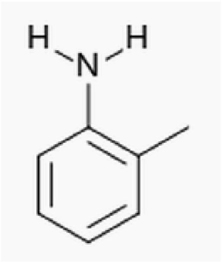
Unfortunately, tests with other red dyes did not inhibit knock, disproving the theory.

But, finding powerful antiknock additives was a major serendipitous discovery!

Mayflower – Trailing Arbutus Jane in early spring

Boyd T (1950) Pathfinding in Fuels and Engines. SAE 500175, 4(2) 182-195.

Lessons from history (1920-30) – **Amines and TEL**



Research after WW-I was motivated by national security

- Improved fuel efficiency with higher CRs made possible the first non-stop airplane flight from New York to San Diego in the 1920's.

GM and US Army studied hundreds of additives

- found aromatic amines to be effective knock suppressors.

1920 experimental GM car driven on gasoline with toluidine with CR ~7:1

- 40% better fuel consumption than 4:1.

Engine exhaust plagued by unpleasant odors - "the goat"!

Much research was devoted to find acceptable additives,

- finally leading to tetraethyl lead (TEL)

But, TEL caused solid deposits, damaged exhaust valves and spark plugs.
Scavenger additives with bromine and chlorine corrected the problem.

- Partnership with Ethyl-Dow and DuPont to extract compounds from sea water
- 10 tons of sea water needed to provide 1 lb of bromine!

WW-II aviation engines used iso-heptane (triptane: 2,2,3-trimethyl butane)

- allowed CR as high as 16:1.

Lessons from history (1930-70) – **TEL and the future**

Lead poisoning was an early concern

- In 1926 US Surgeon General determined that TEL poses no health hazards.
- Use of lead in automotive fuels has been called "The mistake of the 20th century"

1950: Dr. Arie Haagen-Smit - cause of smog in LA to be HC/NO

- Cars were the largest source of UHC/NOx

1950: Eugene Houdry - developed catalytic converter for auto exhaust.

- But, lead was found to poison catalytic converters.

20 years later: US EPA announces gas stations must offer "unleaded" gasoline,

- Based accumulated evidence of negative effects of lead on human health.
- Leaded gasoline was still tolerated in certain applications (e.g., aircraft), but was permanently banned in the US in 1996, in Europe since 2000

World Wars & national security played a major role to define automotive fuels.

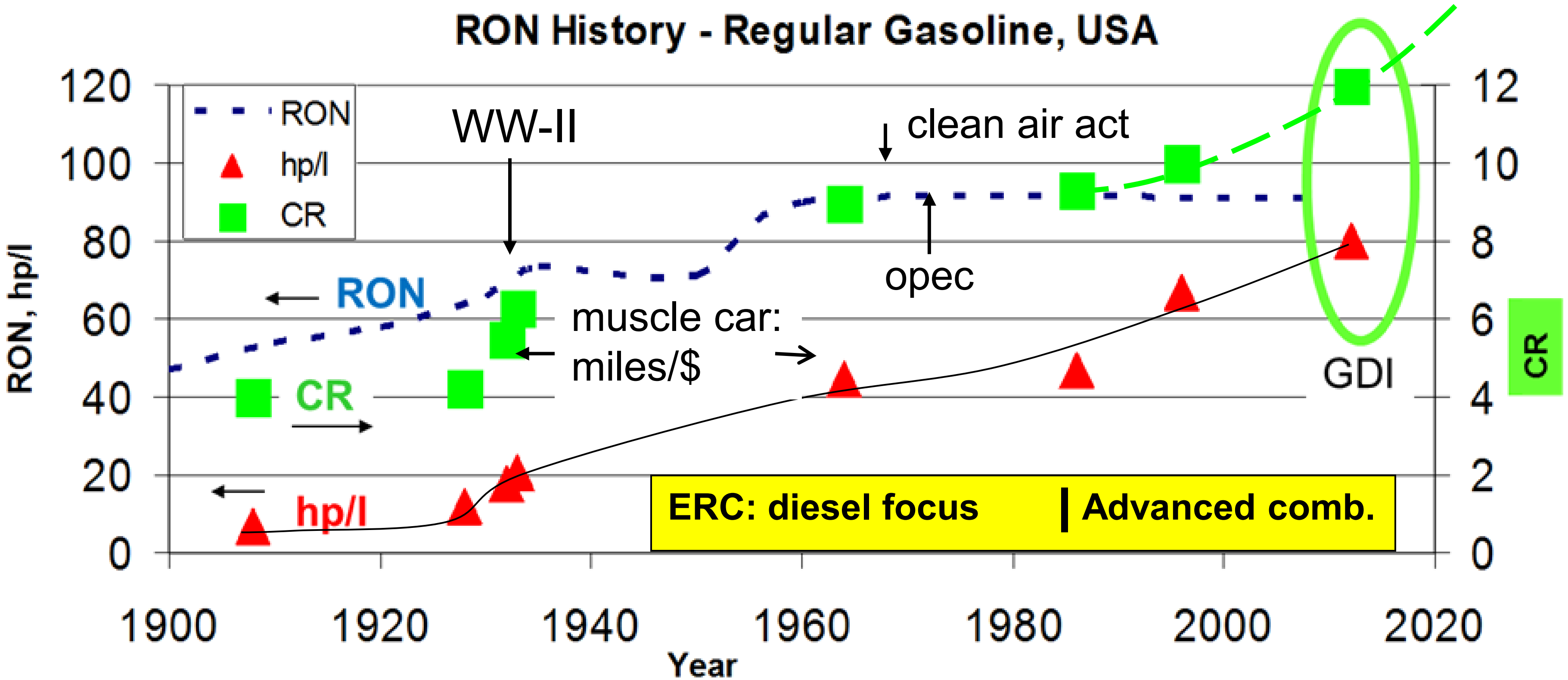
Today's engines and their fuels would not have been developed without close collaboration between engine OEMs, energy and chemical companies!

A consequence of collaboration between "big" engine and "big" oil is that transformative changes in transportation systems will not occur easily.

→ A new concept engine must be able to use available fuels,
A new fuel must run in existing engines.

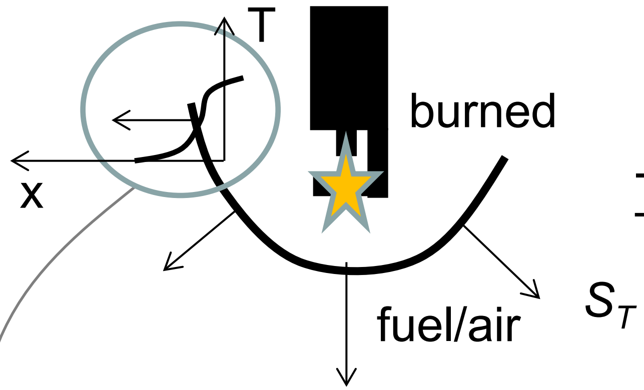
"Race between compression ratio and octane number"

Curtis, 2013



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:

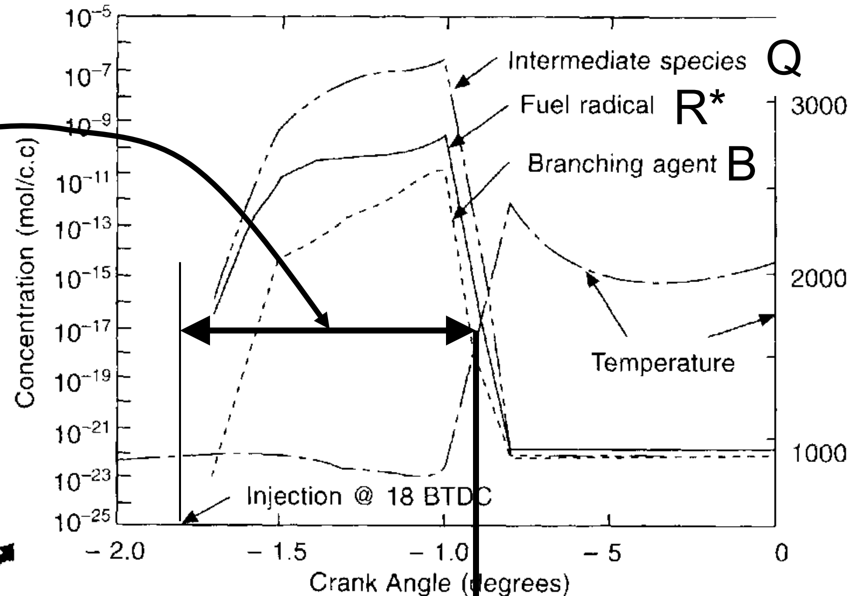
$$\boxed{S_T = \sqrt{D \frac{dY_i}{dt}} \sim V_{piston}}$$

Glassman, 1996

Halstead, 1977

Basic combustion concepts – Diesel (CI)

Ignition Delay

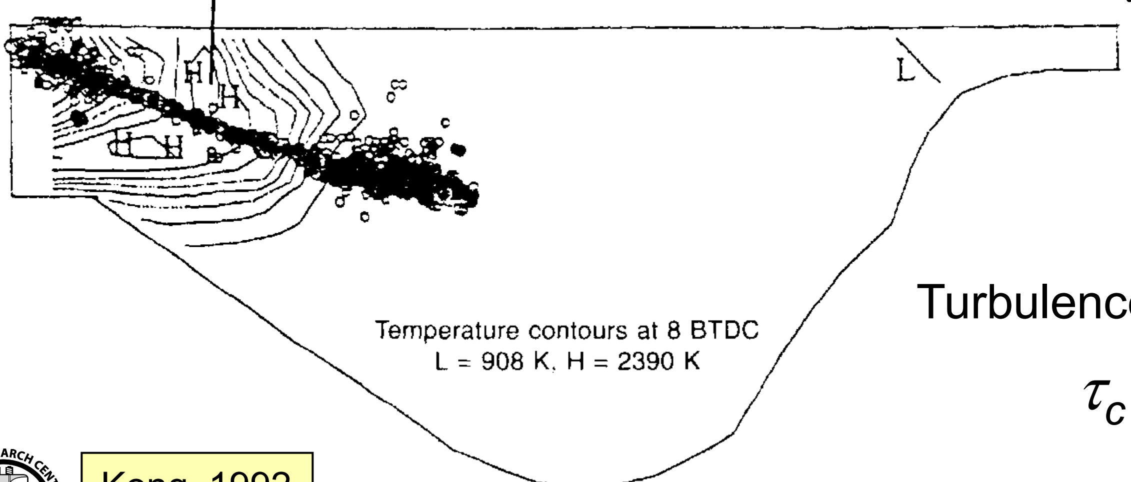


Shell Ignition Model

$RH + O_2$	→	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

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



Temperature contours at 8 BTDC
L = 908 K, H = 2390 K

Turbulence generated by fuel injection

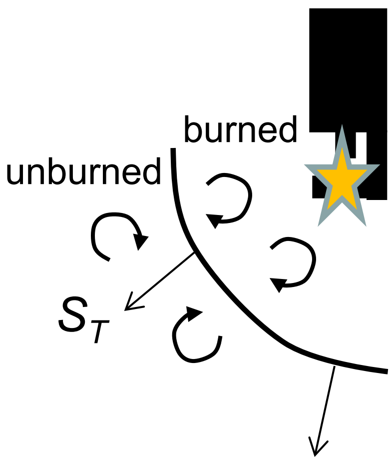
$$\tau_c \sim k/\varepsilon \sim L_{nozzle} \;/\; V_{nozzle}$$

Kong, 1992

Turbulent mixing

Spark-ignition

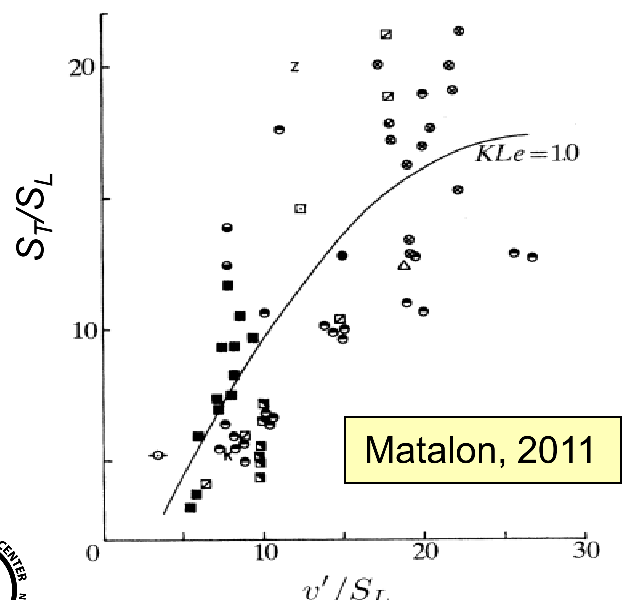
Hot products with
Cold reactants

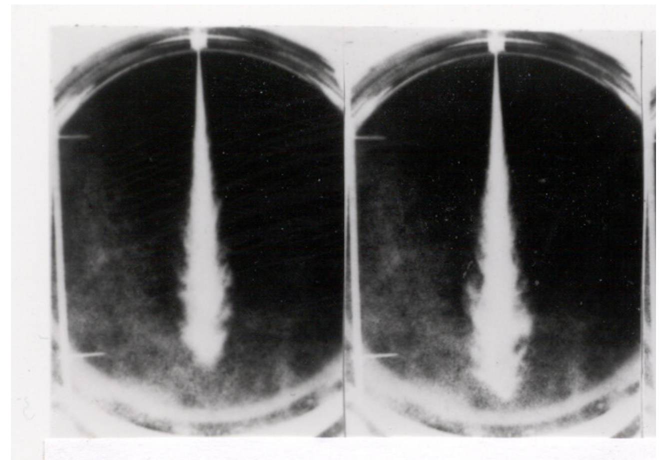


$\tau \sim k/\varepsilon$

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

High turbulence
- faster combustion



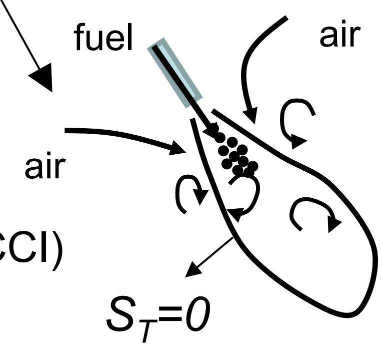


Diesel

Injected fuel with
entrained air

$\tau \sim k/\varepsilon$

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



Delayed ignition (PCCI)
- better mixing

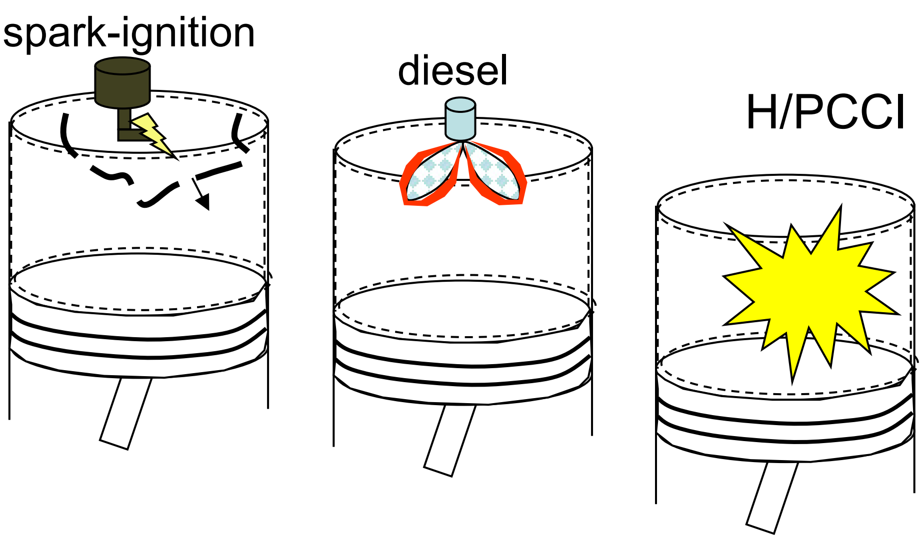
Summary of combustion regimes

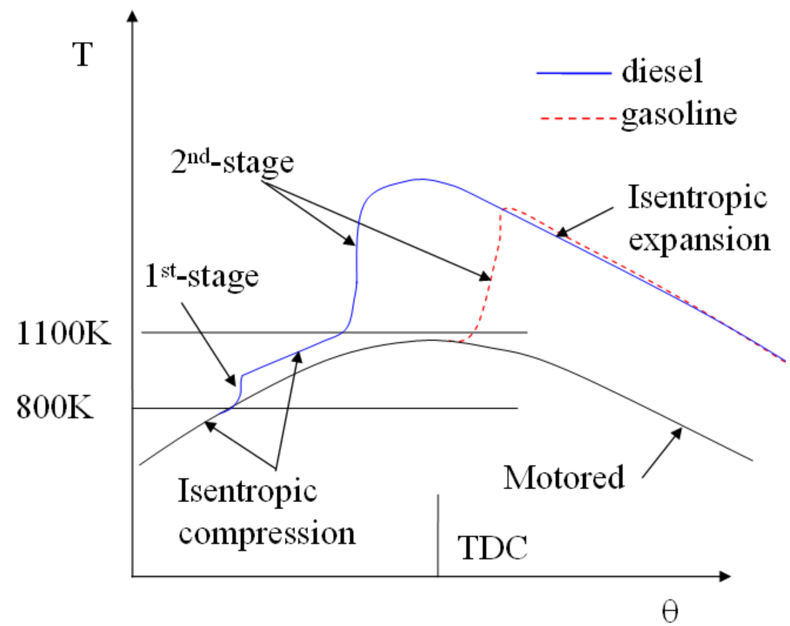
- Gasoline engine spark-ignition with flame propagation:

  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%

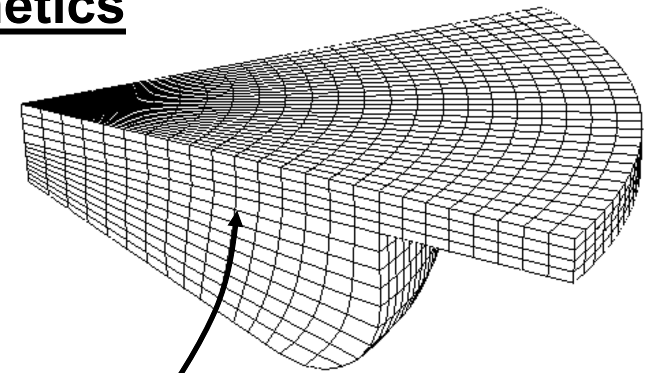




Williams, 1988

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)

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

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

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

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

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

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

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

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

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

Law, 2006,
Warnatz, 2006

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

H_2O_2 chemistry

High temperature

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 $HO_2 + OH \Rightarrow O_2 + H_2O$

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

Methylidyne Reactions

27 $CH + O_2 \Rightarrow CHO + O$

31 $CH + OH \Rightarrow CH_2O + H$

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

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

Law, 2006

Homogeneous charge: no spatial gradients

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

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

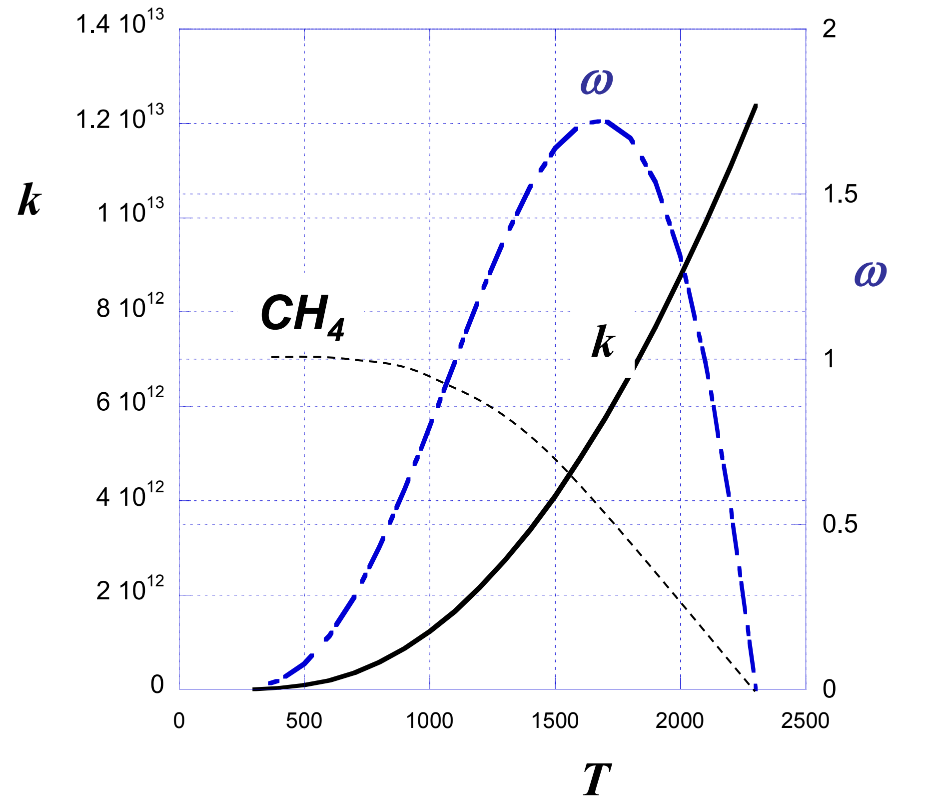
Consider single overall reaction

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

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

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

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



Reitz, 1981

HCCI: Ignition delay

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

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

Consider single component system

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

Example:

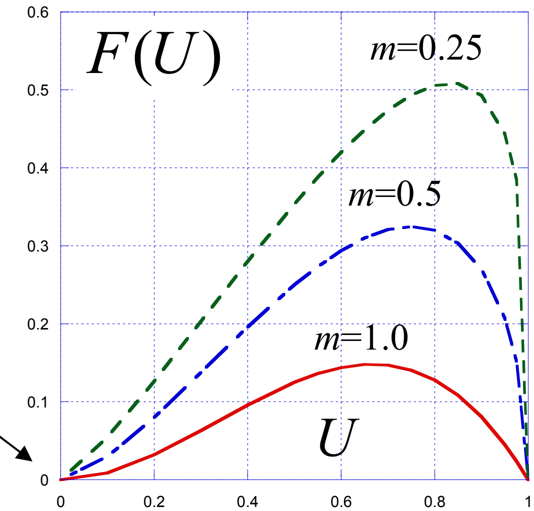
$$\boxed{\frac{dU}{dt} = F(U) = \beta U^{m+1}(1-U)^m}$$

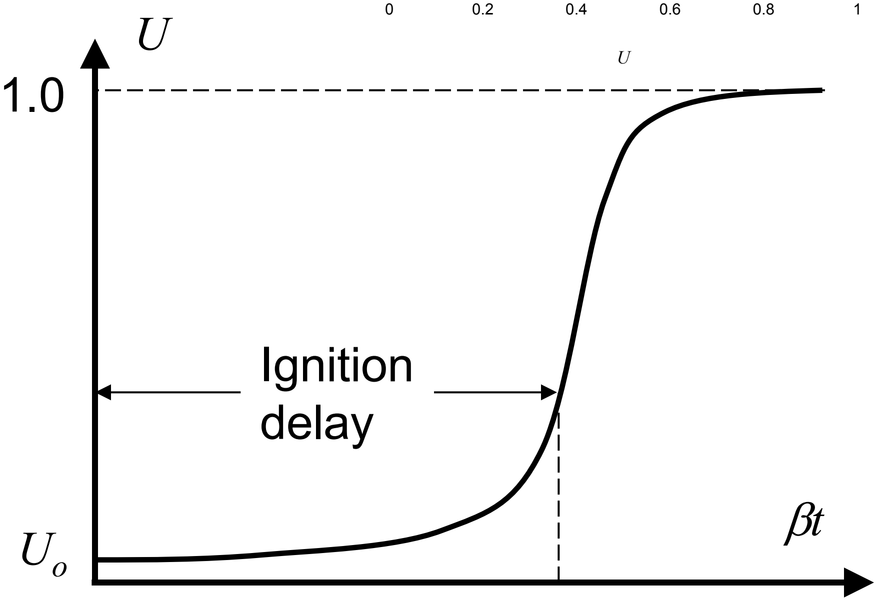
For $U \rightarrow U_o$: $m\beta t = \frac{1}{U_0^m} - \frac{1}{U^m}$

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

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

Cold boundary difficulty





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

Warnatz, 2006

Hydrocarbon kinetics - NTC

Second Stage Ignition

$H_2O_2 = OH + OH$

RH

$\downarrow O_2$

$R^\bullet$ → olefin + R

$\downarrow O_2$

RO_2

$\downarrow$

QOOH → olefin + HO_2
QOOH → cyclic ether + OH

$\downarrow O_2$

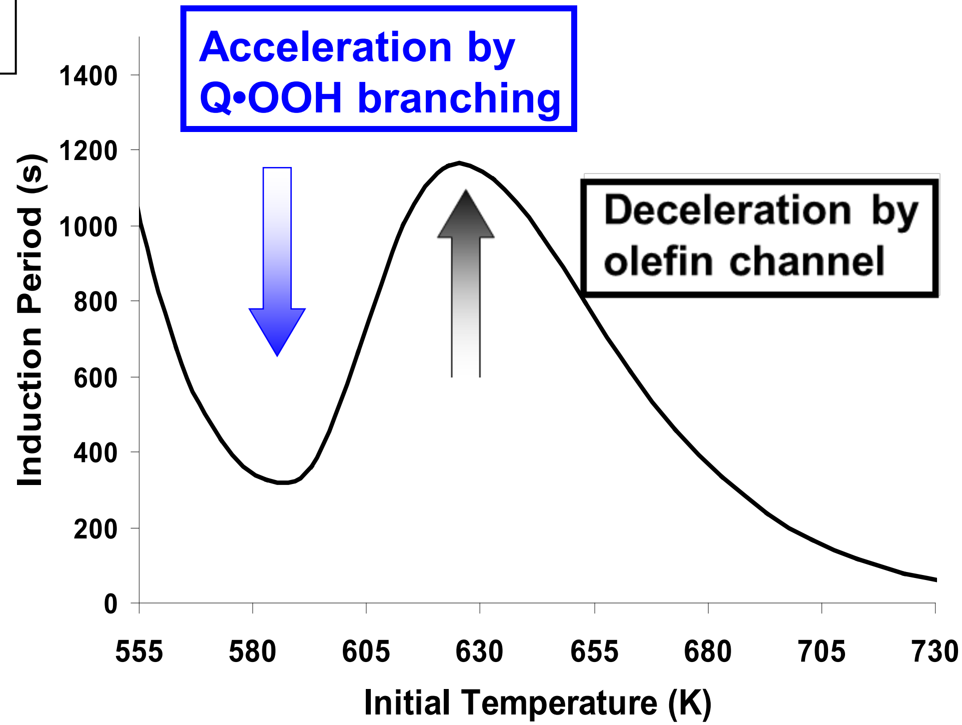
O_2QOOH → keto-hydroperoxide + OH → (low T branching)

deceleration

acceleration

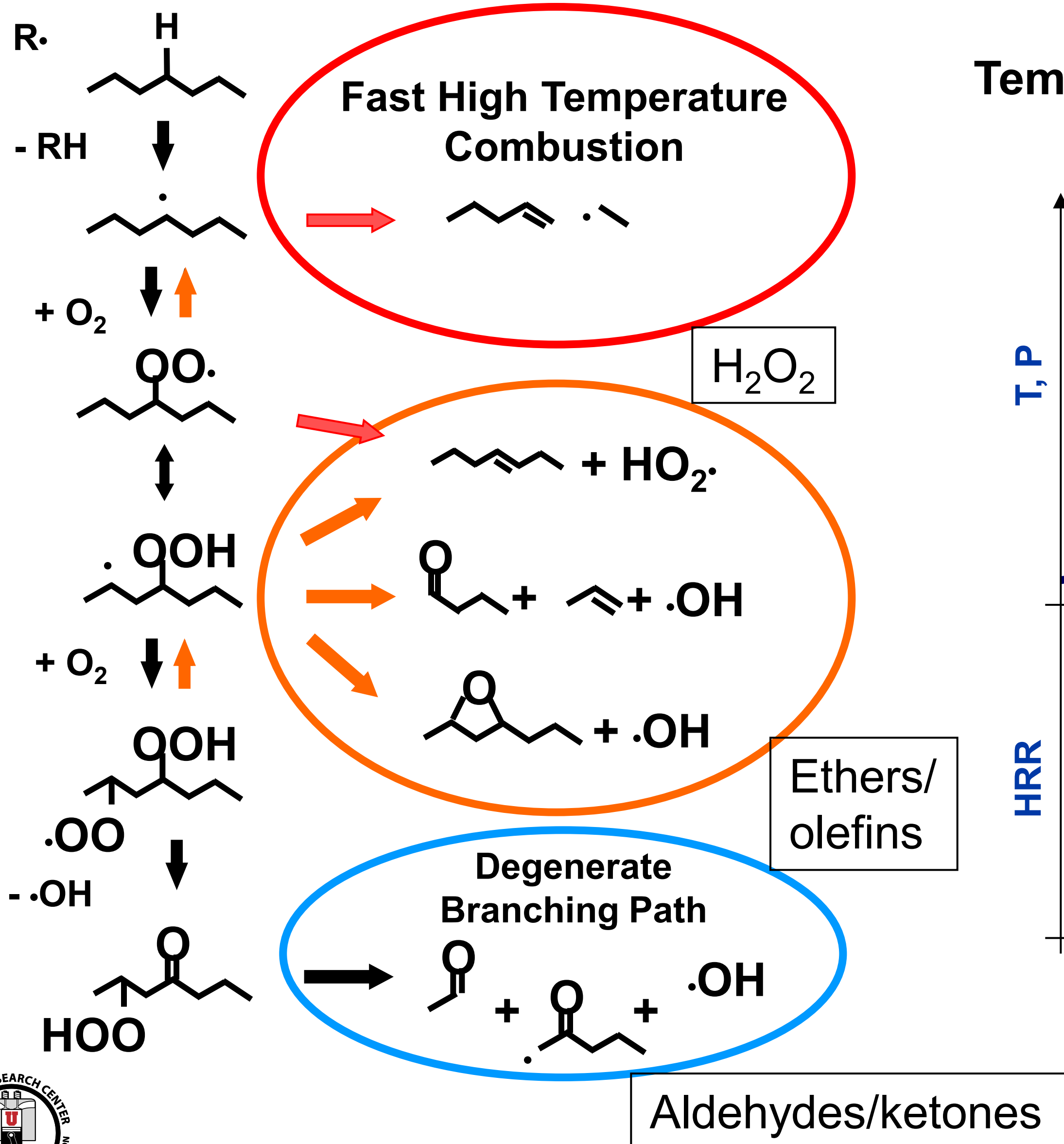
First Stage Ignition

Isomerization steps

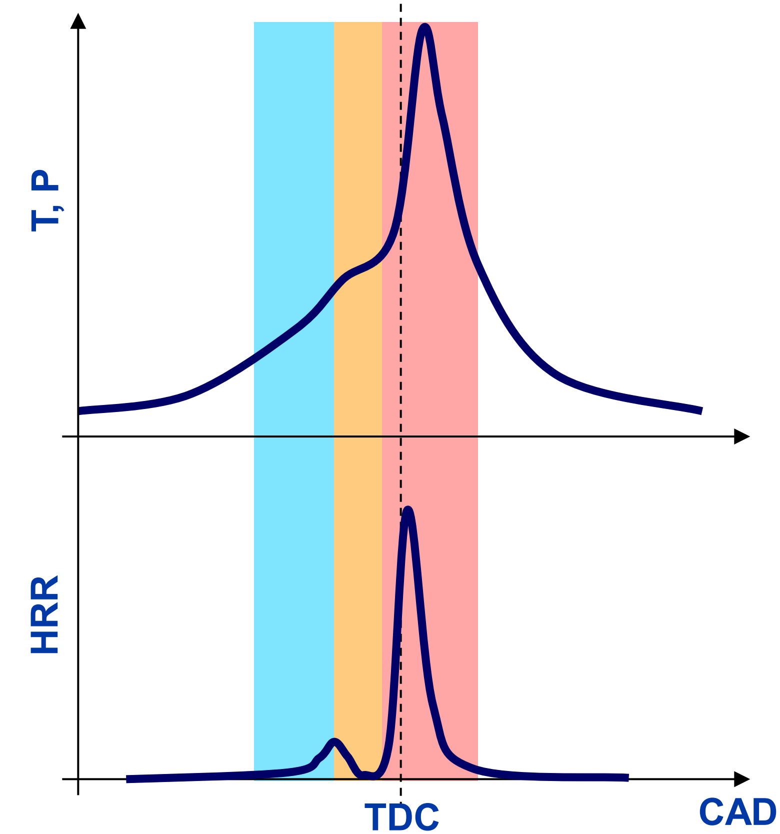


Mehl, 2009

HCCI combustion kinetics



Typical HCCI Combustion Temperature and Heat Release Rate profiles

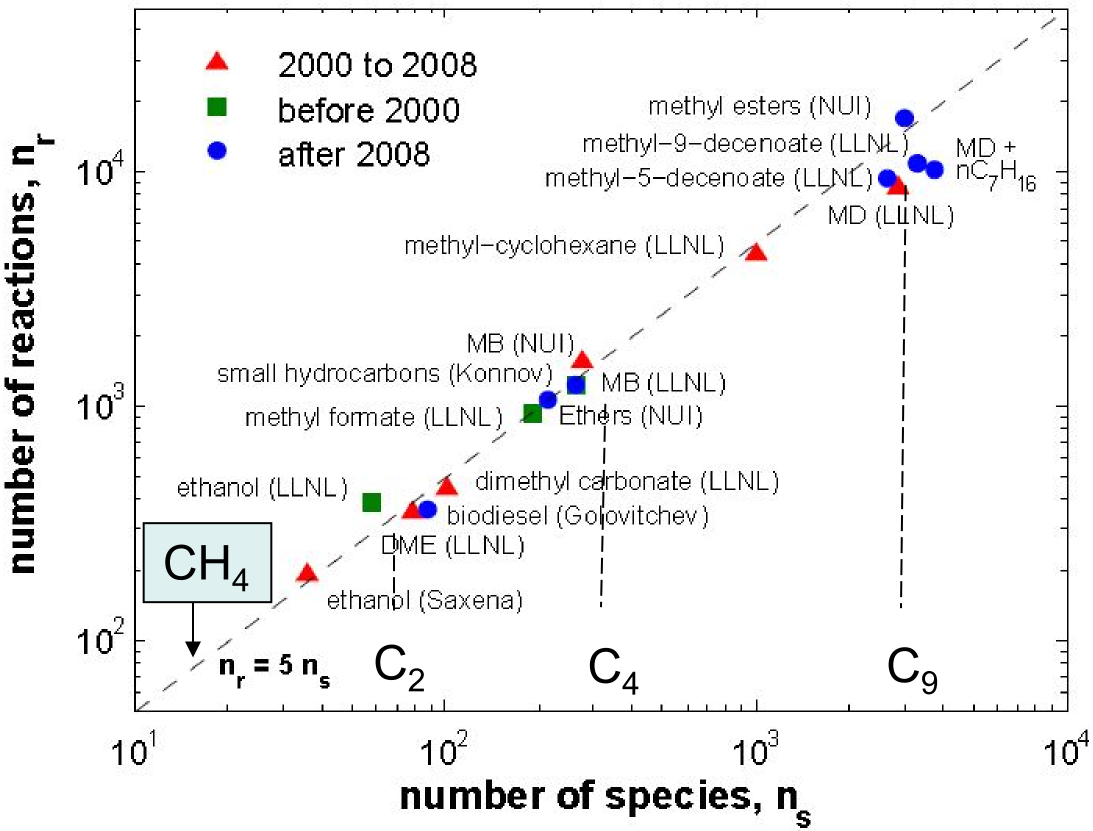


Lu, 2009
Brakora, 2013

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.

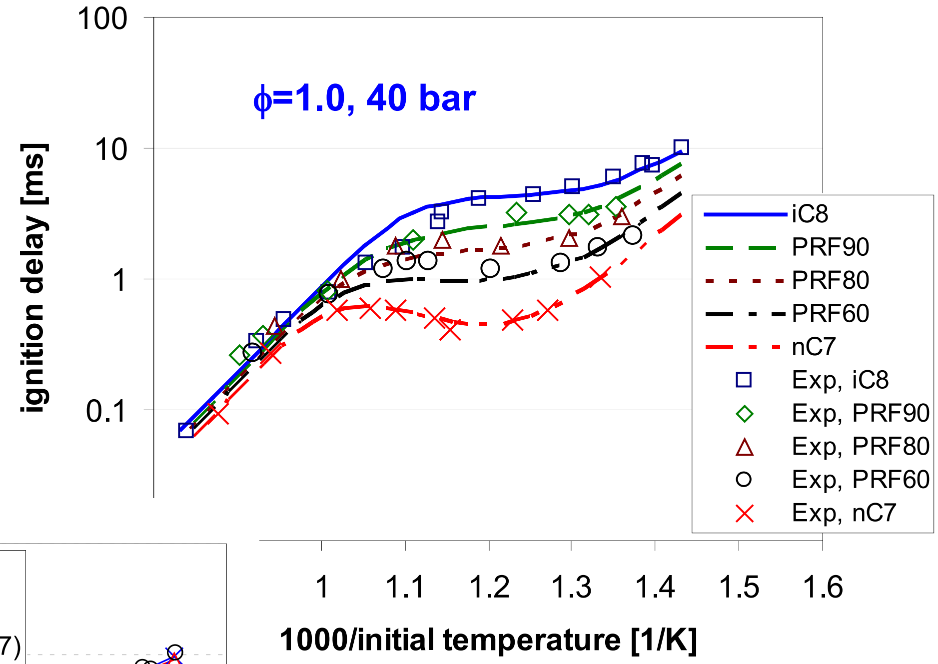
Soy biodiesel - Methyl:
- palmitate (C16:0)
- stearate (C18:0)
- oleate (C18:1)
- linoleate (C18:2)
- linolenate (C18:3)

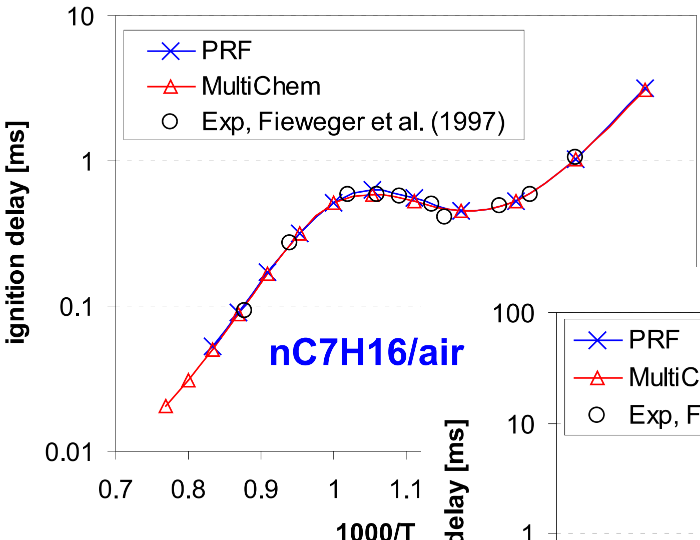
Ra, 2008

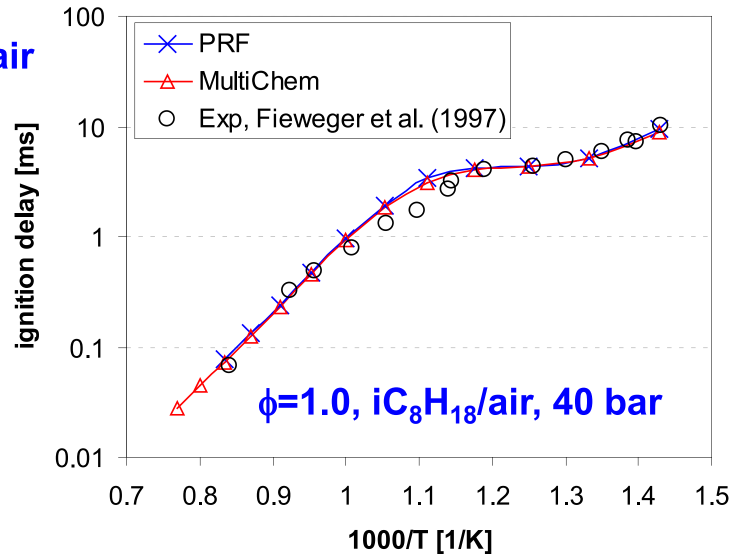
ERC-MultiChem: Primary Reference Fuel (PRF)

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)

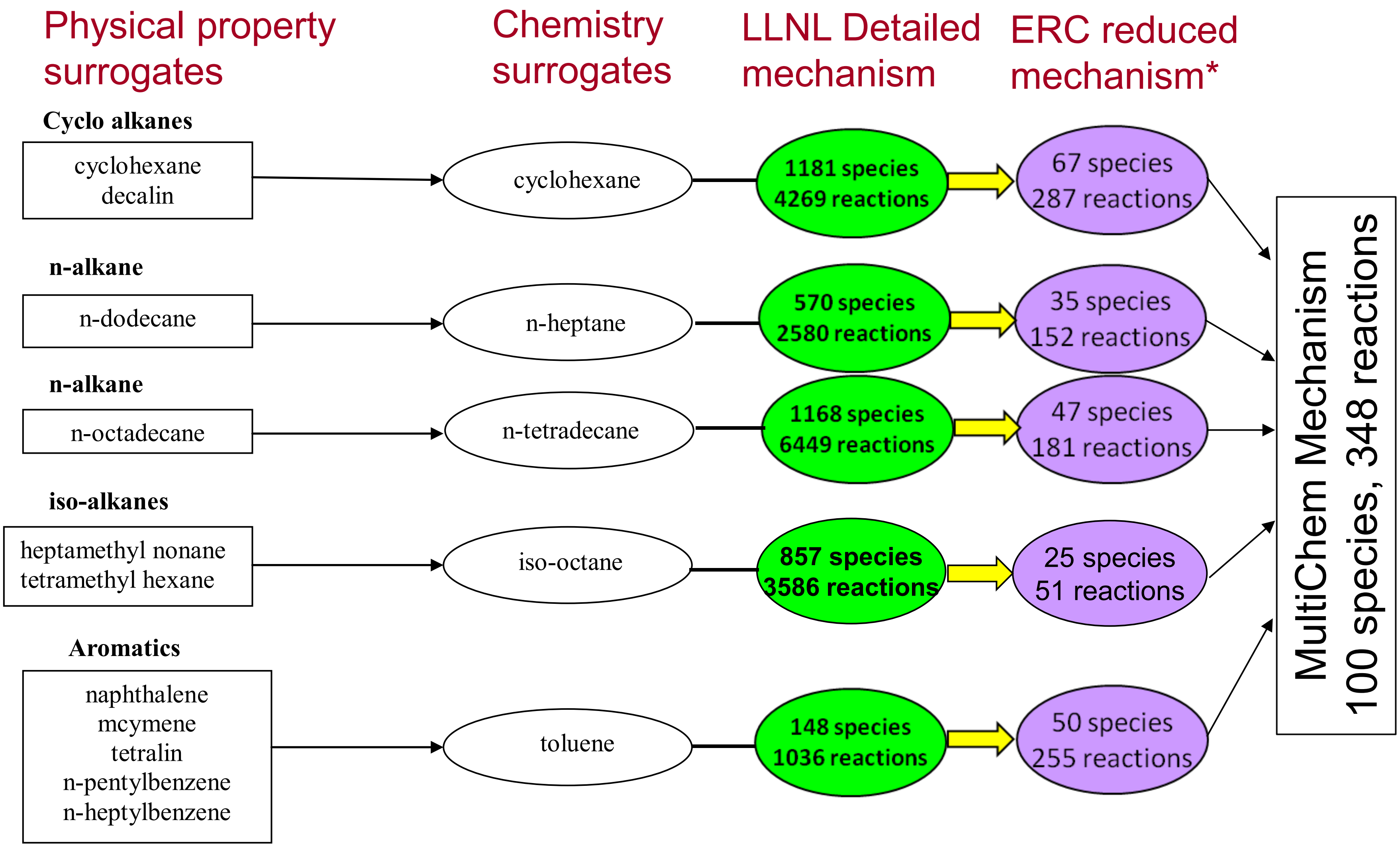






Ra, 2011

Chemical class grouping: "MultiChem" skeletal mechanism

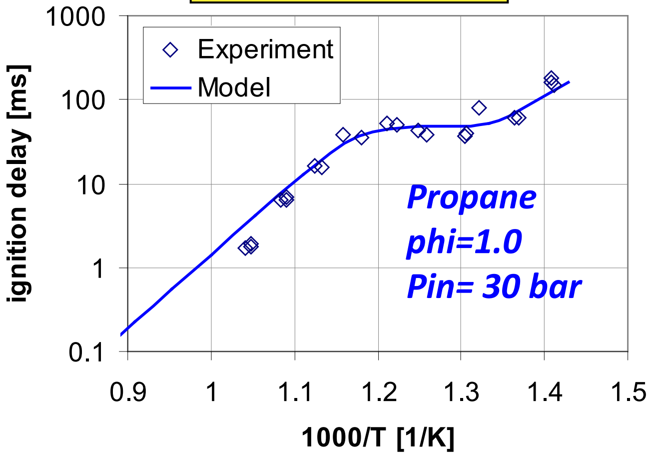


Ra, 2011

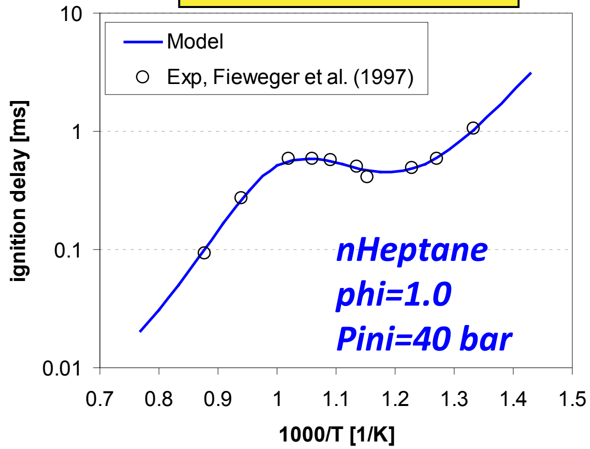
Ignition delay validations - "MultiChem"

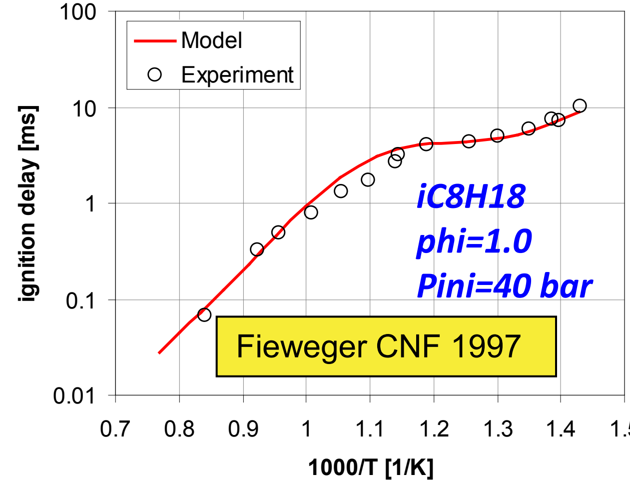
8 Surrogate fuels: *n-heptane, iso-octane, tetradecane, cyclohexane, toluene, decalin, ethanol, MB/D……*

Gauthier CNF 2004

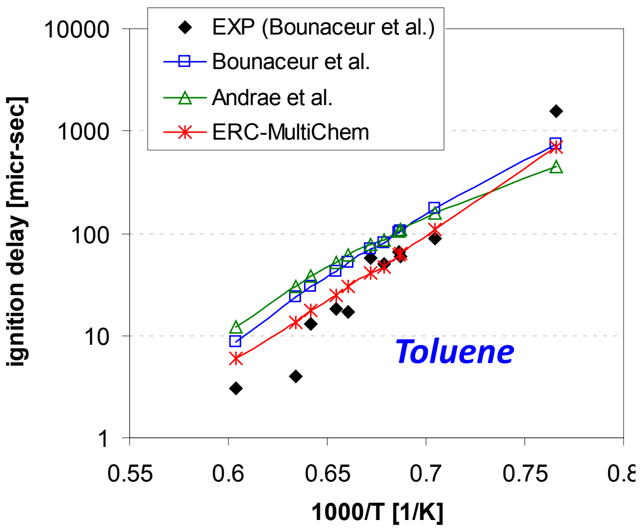


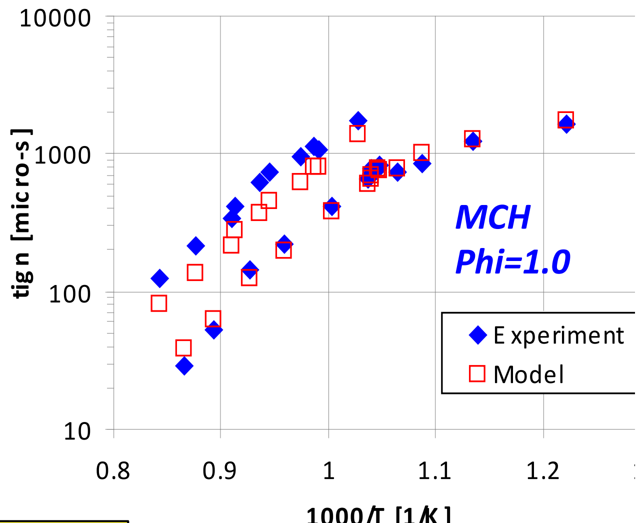
Fieweger CNF 1997

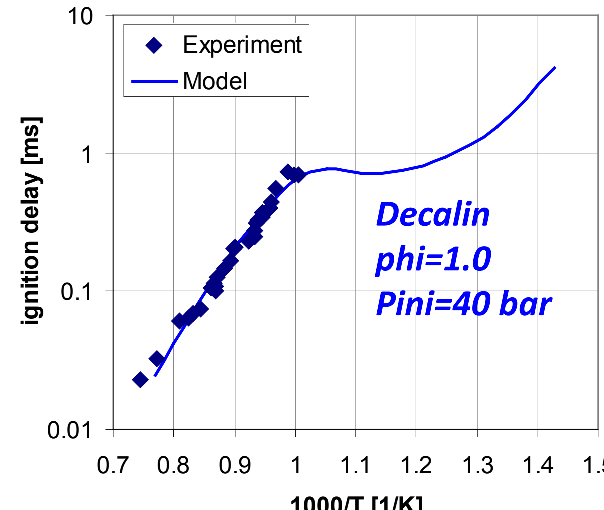




Fieweger CNF 1997







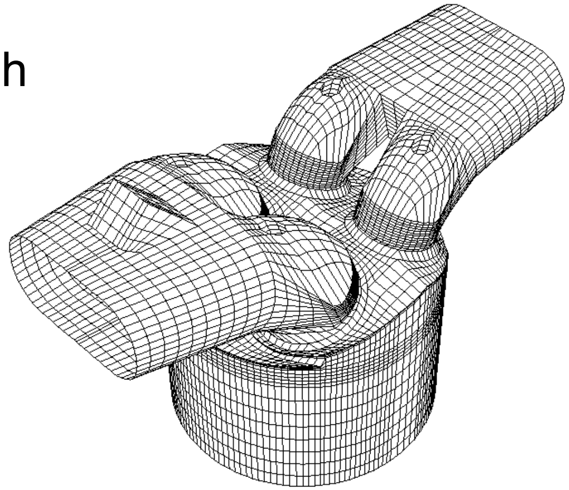
Bounaceur IJCK 2005; Andrae CNF 2005

Shen, Energy & Fuels, 2009

Amsden, 1989, 1997

3-Dimensional models

Solve conservation equations on (moving) numerical mesh



Mass

spray source terms

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

Species

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

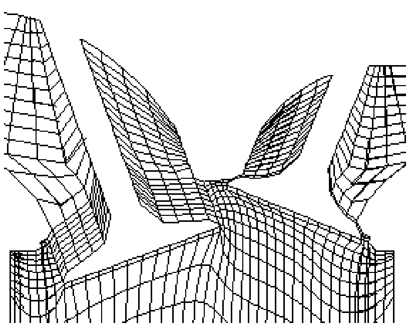
combustion source terms

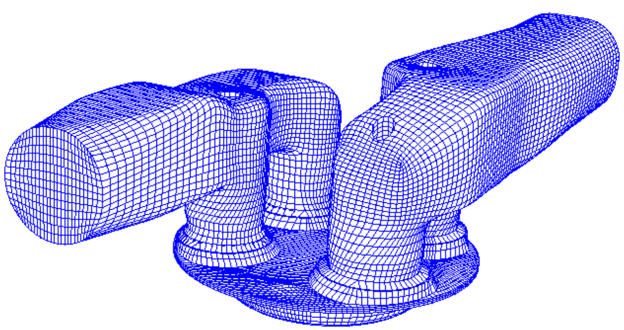
Momentum

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

Energy

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

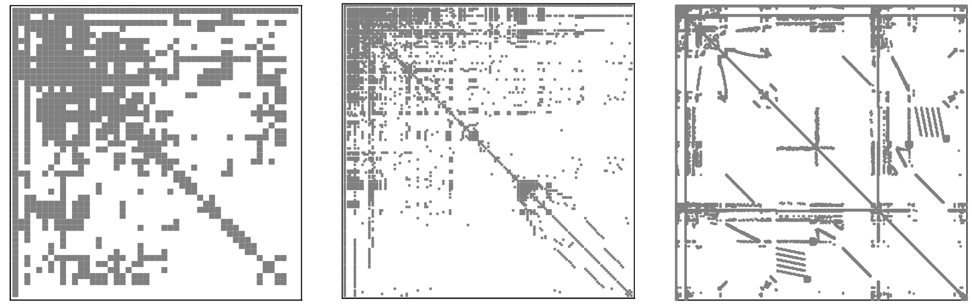




3-D CFD: Improved solver numerics

Sparse analytical Jacobian formulation

Sparsity of hydrocarbon fuel mechanisms increases with size



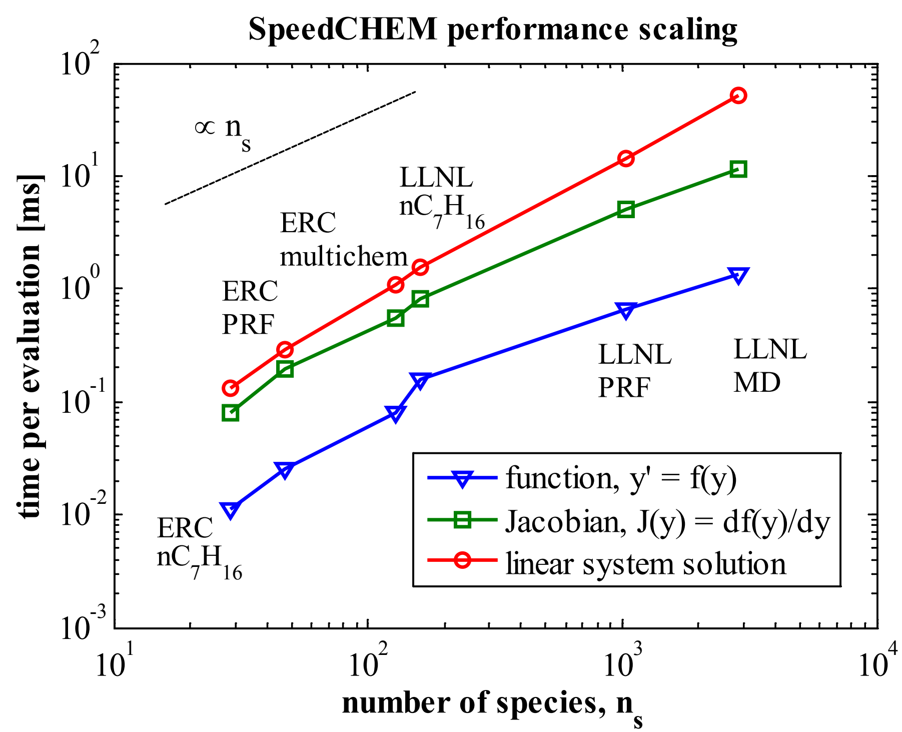
n_s

47 (62.7%) 160 (86.2%) 2878 (99.7%)

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

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

$$\mathbf{J} = \begin{bmatrix} ④\ \dfrac{\partial \dot{T}}{\partial T} & \partial \dot{T}/\partial Y_j\ ② \\ \dfrac{\partial \dot{Y}_i}{\partial T}\ ③ & \dfrac{\partial \dot{Y}_i}{\partial Y_j}\ ① \end{bmatrix}$$



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

Liang, 2009

Shi, 2012
Perini, 2014

Efficient chemistry solvers – cell clustering

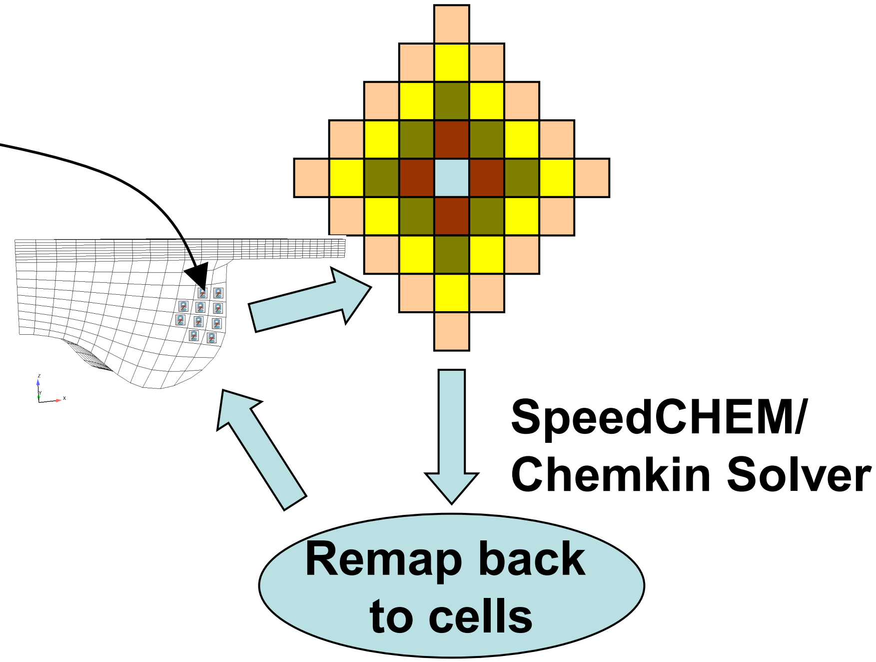
Group thermodynamically-similar cells to reduce the calling frequency to save computer time - Adaptive Mechanism Clustering (AMC) scheme

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)

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

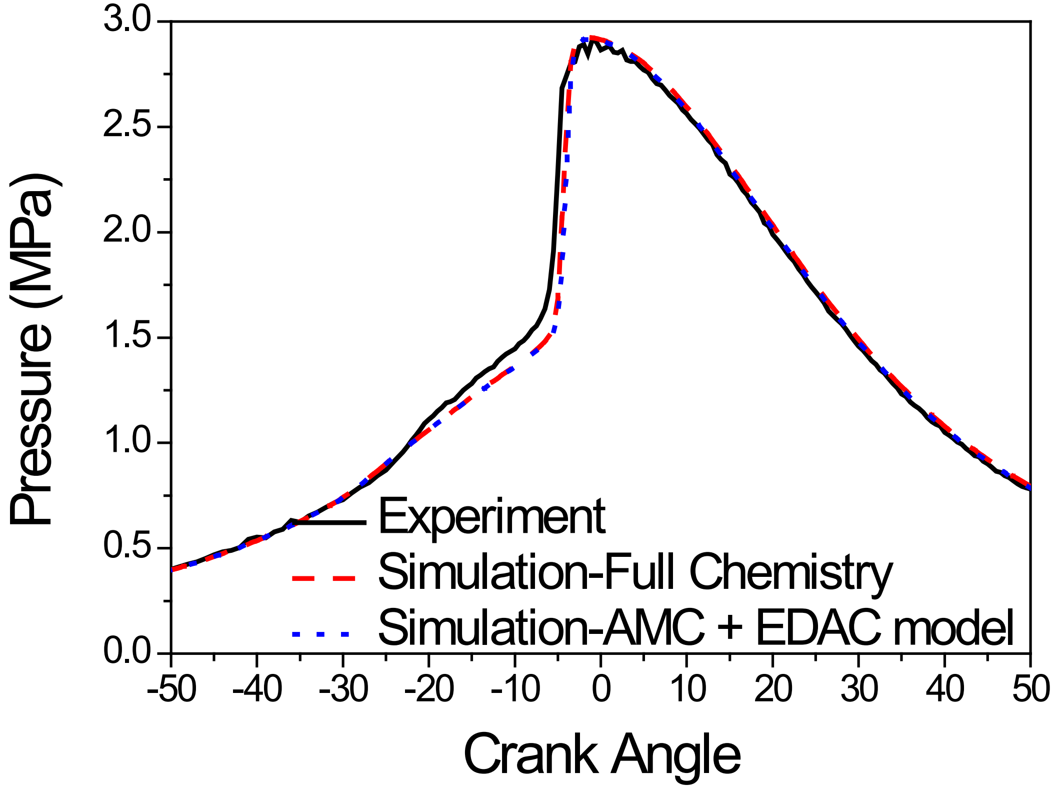


Shi, 2012

HCCI engine validation

ERC PRF mech.
(39 sp, 141 rxn)

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



Engine emissions - transportation & toxic air pollutants

Criteria air contaminants (CAC), or criteria pollutants
- air pollutants that cause smog, acid rain and other health hazards.

EPA sets standards on:

1.) Ozone (O3),
2.) Particulate Matter (soot):
  PM10, coarse particles: 2.5 micrometers (μm) to 10 μm in size
  PM2.5, fine particles: 2.5 μm in size or less
3.) Carbon monoxide (CO), 4.) Sulfur dioxide (SO2),
5.) Nitrogen oxides (NOx), 6.) Lead (Pb)

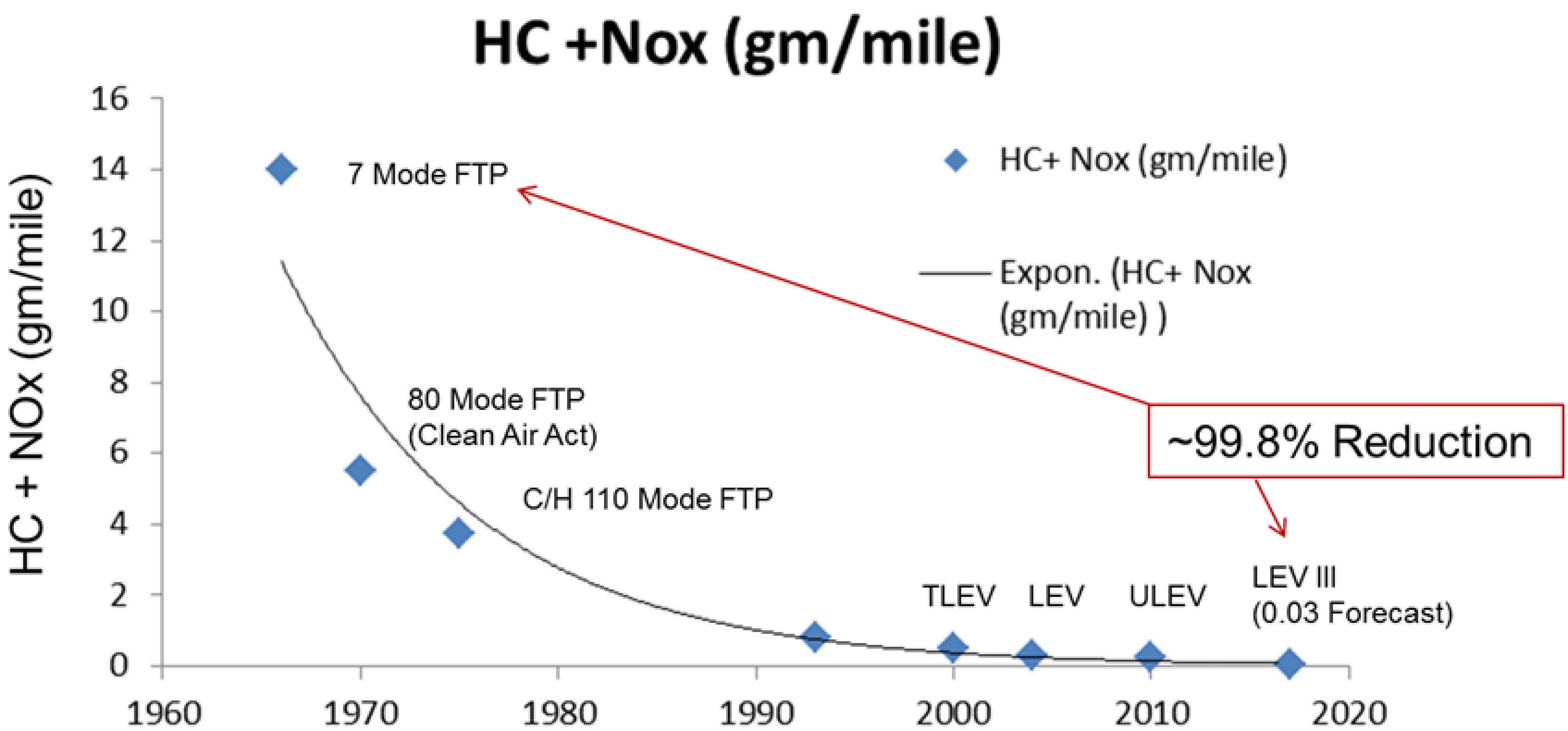
Toxic air pollutants - Hazardous Air Pollutants or HAPs known to cause or suspected of causing cancer or other serious health ailments.
- Clean Air Act Amendments of 1990 lists 188 HAPs from transportation.

In 2001, EPA issued Mobile Source Air Toxics Rule:
- identified 21 MSAT compounds.
- a subset of six identified having the greatest influence on health:
  benzene, 1,3-butadiene, formaldehyde, acrolein, acetaldehyde, and diesel particulate matter (DPM).

Harmful effects on the central nervous system:
BTEX/N/S - benzene, toluene, ethylbenzene, xylenes, Naphthalene, Styrene

Engine emissions - transportation & toxic air pollutants

Future emissions standards will be a challenging constraint.



Yoshikawa, 2008

NOx modeling

Zeldo'vich thermal NOx mechanism

$$O + N_2 <=> NO + N$$ ← Rate controlling step due to high N_2 bond strength

$$N + O_2 <=> NO + O$$

$$N + OH <=> NO + H$$

ERC 12-step NOx model is based on GRI-Mech v3.11 and includes:

- Thermal NOx — Zeldovich, 1946
- Prompt NOx around 1000 K. — Fenimore, 1979

Extensions

- NO can convert HCN and NH_3 — Eberius, 1987
- Interaction between NO and Soot — Guo, 2007

Summary

IC engine combustion physics depends critically on fuel chemistry

Much progress has been made in understanding and modeling combustion chemistry for realistic fuels

The various combustion regimes require different fuels, with differences in autoignition characteristics playing a major role

Meeting future toxic emissions regulations will require significant advances in engine research

References

2-4:3 http://www.erc.wisc.edu/combustion.php

2-4:4 Park, S.W., and Reitz, R.D., "Numerical Study on the Low Emission Window of Homogeneous Charge Compression Ignition Diesel Combustion," Combustion Science and Technology, Vol. 179:11, pp. 2279-2307, 2007.

2-4:5 http://www.erc.wisc.edu/documents/symp13-Daw.pdf

2-4:6 Boyd T (1950) Pathfinding in Fuels and Engines. SAE 500175, 4(2) 182-195

2-4:7-8 Reitz, R.D., "Grand challenges in engine and automotive engineering," Front. Mech. Eng. 1:1, http://journal.frontiersin.org/article/10.3389/fmech.2015.00001/full, 2015

2-4:9,29 Curtis, E., Private communication, 2014

2-4:10 I. Glassman, Combustion, Academic Press, New York, 3rd Ed., 1996

2-4:10 Reitz, R.D. and Bracco, F.V., "Global Kinetics and Lack of Thermodynamic Equilibrium," Comb. Flame, V.53, p.141, 1983.

2-4:10 Abraham, J., Bracco, F.V. and Reitz, R.D. "Comparisons of Computed and Measured Premixed Charge Engine Combustion," Combust. Flame, 60, pp. 309-322, 1985.

2-4:11 Kong, S.-C., Ayoub, N., and Reitz, R.D., "Modeling Combustion in Compression Ignition Homogeneous Charge Engines," SAE Paper 920512, SAE Transactions, Vol. 101, Section 3, Journal of Engines, pp. 896-911,1992.

2-4:11 Halstead, M., Kirsh, L. and Quinn, C. "The Autoignition of Hydrocarbon Fuels at High Temperatures and Pressures - Fitting of a Mathematical Model," Combust. Flame, Vol. 30, pp. 45-60, 1977.

2-4:12 Matalon, 2011 - http://www.princeton.edu/engineering/video/player/?id=5922

2-4:14 F.A. Williams, Combustion Theory, Addison-Wesley Pub., Reading, Mass, 2nd Ed. 1988.

2-4:15-16 C.K. Law, Combustion Physics, Cambridge University Press, 2006.

2-4:15,18 J. Warnatz, U. Maas and R.W. Dibble, "Combustion, Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation" by, Springer, 4th Edition, 2006.

2-4:17 Reitz, R.D., "A Study of Numerical Methods for Reaction-Diffusion Equations," SIAM Journal on Scientific and Statistical Computing, Vol. 2, p. 95, 1981.

2-4:19 Mehl M., T. Faravelli, E. Ranzi, D. Miller,N. Cernansky, “Experimental and kinetic modeling study of the effect of fuel composition in HCCI engines”, Proceedings of the Combustion Institute 32, 2843-2850 (2009)

References

2-4:20 T. F. Lu and C. K. Law, "Toward accommodating realistic chemistry in large-scale computations,“ Progress in Energy and Combustion Science, Vol. 35, pp. 192-215 (2009)

2-4:20 Brakora, J.L., and Reitz, R.D., "A Comprehensive Combustion Model for Biodiesel-fueled Engine Simulations," SAE Paper 2013-01-1099, 2013.

2-4:21-23 Ra, Y., and Reitz, R.D., "A Reduced Chemical Kinetic Model for IC Engine Combustion Simulations with Primary Reference Fuels," Combustion & Flame, Vol. 155, pp. 713–738, 2008.

2-4:23 Fieweger, K., Blumenthal, R., and Adomeit, G. (1997) "Self-Ignition of S.I. Engine Model Fuels: A Shock Tube Investigation at High Pressure," Combustion and Flame, Vol. 109, pp. 599-619.

2-4:23 Ra, Y., and Reitz, R.D., "A Combustion Model for IC Engine Combustion Simulations with Multi-component Fuels," Combustion & Flame, Vol. 158, pp. 69-90, 2011.

2-4:23 B.M. Gauthier, D.F. Davidson, R.K. Hanson, Combust. Flame 139 (2004) 300–311.

2-4:23 R. Bounaceur, I. Da Costa, R. Fournet, F. Billaud, F. Battin-Leclerc “Experimental and Modeling Study of the Oxidation of Toluene,” Int. J. Chem. Kinet. 37 (2005) 25–49.

2-4:23 J. Andrae, D. Johansson, P. Björnbom, P. Risberg, G.T. Kalghatgi, Combust. Flame 140 (2005) 267-286.

2-4:23 H-P. S. Shen, J. Steinberg, J. Vanderover, M. A. Oehlschlaeger, Energy & Fuels 23 (2009) 2482–2489.

2-4:24 Amsden, A.A. (1997) KIVA-3V: A block-structured KIVA program for engines with vertical or canted valves. Los Alamos National Laboratory Report No. LA-13313-MS.

2-4:25,26 Perini, F., Das Adhikary, B., Lim, J.H., Su, X., Ra, Y., Wang, H., and Reitz, R.D., "Improved Chemical Kinetics Numerics for the Efficient Simulation of Advanced Combustion Strategies," Int. J. Engines 7(1):2014.

2-4:26 Liang, L., Steven, J.G., Farrell, J.T., “A dynamic adaptive chemistry scheme for reactive flow computations,” Proc. Combustion Inst. 32:527-534, 2009

2-4:26,27 Shi, Y., Ge, H.-W, and Reitz, R.D., “Computational Optimization of Internal Combustion Engines,” ISBN 978-0-85729-618-4, Springer, 2011 http://www.springer.com/engineering/mechanical+eng/book

References

2-4:30 Yoshikawa, T., and Reitz, R.D., "Development of an Improved NOx Reaction mechanism for Low Temperature Diesel Combustion Modeling," SAE 2008-01-2413, SAE Int. J. Engines, Vol. 1(1), pp. 1105-1117, 2009.

2-4:30 Zeldovich, Y. B., "The oxidation of nitrogen in combustion and explosions," Acta Physicochim, USSR 21:577, 1946.

2-4:30 Fenimore, C. P., "Studies of fuel-nitrogen in rich flame gases," Proceeding of Combustion Institute, 17:661, 1979.

2-4:30 Eberius, H., Just, T., Kelm, S., Warnatz, J., and Nowak, U., "Konversion von brennstoffgebundenem Stickstoff am Beispiel von dotierten Propan-Luft-Flammen," VDI-Berichte, 645:626, 1987.

2-4:30 Guo, H., and Smallwood, G. J., "The interaction between soot and NO formation in a laminar axisymmetric coflow ethylene/air diffusion flame," Combustion and Flame, 149, pp. 225-233, 2007.