Hour 4: Engine combustion physics and chemistry

Internal Combustion Engines I: Fundamentals and Performance Metrics

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

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
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.
IC Engine combustion regimes

Kamimoto plot

PCCI – Premixed Charge Compression Ignition
HCCI – Homogeneous Charge Compression Ignition

Conventional diesel

Early injection PCCI

Part 5: Diesel and SI Engine combustion

Park, 2007
Advanced combustion regimes

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

Low (e.g., gasoline) Prevents Auto-Ignition
Fuel Reactivity
High (e.g., diesel) Promotes Auto-Ignition
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!
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”

RON History - Regular Gasoline, USA

- RON: Reid Octane Number
- hp/l: Horsepower per Liter
- CR: Compression Ratio

Key Events:
- WW-II
- Clean Air Act
- OPEC

 ERC: Diesel focus
Advanced comb.

Year:
- 1900
- 1920
- 1940
- 1960
- 1980
- 2000
- 2020

Curtis, 2013
Basic combustion concepts – Spark Ignition (SI)

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

Because turbulent flame speed, $S_T$, scales with rpm!

Kinetic energy, $k \sim V_{piston}^2$

Integral length scale $l_i \sim L_{piston}$

Kinetic energy dissipation rate, $\epsilon \sim V_{piston}^3 / L_{piston}$

Diffusivity, $D \sim k^2 / \epsilon \sim V_{piston} L_{piston}$

Characteristics Time Combustion (CTC) model

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

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

Mallard-Le Chatelier propagating wave speed:

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

Glassman, 1996

Reitz & Bracco, 1983; Abraham, 1985
Basic combustion concepts – Diesel (CI)

Shell Ignition Model

\[ \text{RH} + \text{O}_2 \rightarrow 2\text{R}^* \]

\[ \text{R}^* \rightarrow \text{R}^* + \text{P} + \text{Heat} \]

\[ \text{R}^* \rightarrow \text{R}^* + \text{B} \]

\[ \text{R}^* \rightarrow \text{R}^* + \text{Q} \leftarrow \text{Af04} \]

\[ \text{R}^* + \text{Q} \rightarrow \text{R}^* + \text{B} \]

\[ \text{B} \rightarrow 2\text{R}^* \]

\[ \text{R}^* \rightarrow \text{termination} \]

\[ 2\text{R}^* \rightarrow \text{termination} \]

Switch to Characteristic Time Combustion model

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

Turbulence generated by fuel injection

\[ \tau_c \sim \frac{k}{\varepsilon} \sim \frac{L_{\text{nozzle}}}{V_{\text{nozzle}}} \]

Ignition Delay

Temperature contours at 8 BTDC

\[ L = 908 \text{ K} \]

\[ H = 2390 \text{ K} \]

Kong, 1992

Halstead, 1977
**Turbulent mixing**

**Spark-ignition**

- Hot products with Cold reactants

\[ \tau \sim \frac{k}{\varepsilon} \]
\[ \sim \frac{L_{\text{piston}}}{V_{\text{piston}}} \]

- High turbulence - faster combustion

**Diesel**

- Injected fuel with entrained air

\[ \tau \sim \frac{k}{\varepsilon} \]
\[ \sim \frac{L_{\text{nozzle}}}{V_{\text{nozzle}}} \]

- Delayed ignition (PCCI) - better mixing

**Matalon, 2011**
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%
Premixed volumetric combustion & chemical kinetics

Species and energy conservation equations

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

\[ \frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho u I) = -p \nabla \cdot u - \nabla \cdot J + \rho \varepsilon + \dot{Q}^c + \dot{Q}^s + \dot{Q}^v \]

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

\[ \frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} (v^r_{k,i} - v^s_{k,i}) \omega_k (Y, T), \quad i = 1, \ldots, n_s \]

\[ \omega_k (Y, T) = \kappa_{f,k} \prod_{i=1}^{n_s} \left( \frac{\rho Y_i}{W_i} \right)^{v_{k,i}} - \kappa_{b,k} \prod_{i=1}^{n_s} \left( \frac{\rho Y_i}{W_i} \right)^{v_{k,i}} \]

\[ \kappa_{f,k} (T) = A_k T^{b_k} \exp \left( -\frac{E_k}{RT} \right) ; \quad \kappa_{b,k} (T) = \kappa_{f,k} (T) / K_{c_{eq,k}} (T) \]

\[ K_{c_{eq,k}} (T) = \exp \left( -\Delta g_k^0 \right) \left( \frac{p_{atm}}{RT} \right) \sum_{i=1}^{n_s} (v^r_{k,i} - v^s_{k,i}) \]

\[ \frac{dT}{dt} (Y, T) = -\frac{1}{c_v (Y, T)} \sum_{i=1}^{n_s} \left( \frac{e_i (T)}{W_i} \frac{dY_i}{dt} (Y, T) \right) \]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( W_i )</td>
<td>molecular weight</td>
</tr>
<tr>
<td>( Y_i )</td>
<td>mass fraction</td>
</tr>
<tr>
<td>( v^r_{k,i} v^s_{k,i} )</td>
<td>reactant/product stoichiometric coefficients</td>
</tr>
<tr>
<td>( n_r )</td>
<td>reactions</td>
</tr>
<tr>
<td>( n_s )</td>
<td>species</td>
</tr>
<tr>
<td>( I )</td>
<td>specific internal energy</td>
</tr>
<tr>
<td>( M_i )</td>
<td>chemical label</td>
</tr>
<tr>
<td>( K_{c_{eq,k}} )</td>
<td>stoichiometric coefficients</td>
</tr>
<tr>
<td>( e_i )</td>
<td>species energy</td>
</tr>
</tbody>
</table>

\[ e_i = R_{mol} \left[ (a_i - 1) T + \frac{b_i}{2} T^2 + \frac{c_i}{3} T^3 + \frac{d_i}{4} T^4 + \frac{e_i}{5} T^5 + f_i \right] \]
Combustion chemistry models – CH₄ (15 spec, 31 react.)

CH₄ + 2 O₂ = CO₂ + 2 H₂O

Hydrogen-Oxygen Chain
1  H + O₂ ⇌ OH + O
2  H₂ + O ⇌ OH + H
3  H₂ + OH ⇌ H₂O + H
4  H₂O + O ⇌ 2 OH

Hydroperoxyl Formation and Consumption
5b  H + O₂ + M ⇌ HO₂ + M
6  HO₂ + H ⇌ 2 OH
7  HO₂ + H ⇌ H₂ + O₂
8  HO₂ + H ⇌ H₂O + O
9  HO₂ + OH ⇌ O₂ + H₂O

Conversion of Carbon Monoxide to Carbon Dioxide
10 CO + OH ⇌ CO₂ + H

Methane Consumption
11 CH₄ + H ⇌ H₂ + CH₃
12 CH₄ + OH ⇌ H₂O + CH₃

Methyl Reactions
13 CH₃ + O ⇌ CH₂O + H
14 CH₃ + OH ⇌ CH₂O + H + H
15 CH₃ + OH ⇌ CH₂O + H₂
16c CH₃ + H ⇌ CH₄
23 CH₃ + H ⇌ CH₂ + H₂
28 CH₃ + OH ⇌ CH₂ + H₂O

Hydroperoxyl Formation and Consumption
5b  H + O₂ + M ⇌ HO₂ + M
6  HO₂ + H ⇌ 2 OH
7  HO₂ + H ⇌ H₂ + O₂
8  HO₂ + H ⇌ H₂O + O
9  HO₂ + OH ⇌ O₂ + H₂O

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15 CH₃ + OH ⇌ CH₂O + H₂
16c CH₃ + H ⇌ CH₄
23 CH₃ + H ⇌ CH₂ + H₂
28 CH₃ + OH ⇌ CH₂ + H₂O

Formaldehyde Reactions
17 CH₂O + H ⇌ CHO + H₂
18 CH₂O + OH ⇌ CHO + H₂O

Formyl Reactions
19 CHO + H ⇌ CO + H₂
20 CHO + OH ⇌ CO + H₂O
21 CHO + O₂ ⇌ CO + HO₂
22 CHO + M ⇌ CO + H + M

Methylene Reactions
24 CH₂ + O₂ ⇌ CO₂ + H₂
25 CH₂ + O₂ ⇌ CO + OH + H
26 CH₂ + H ⇌ CH + H₂
29 CH₂ + OH ⇌ CH₂O + H
30 CH₂ + OH ⇌ CH + H₂O

Conversion to products by sequential fragmentation by H abstraction
Homogeneous charge: no spatial gradients

\[ \frac{\partial Y_i}{\partial t} = \frac{\omega_i}{\rho} \]

\[ \frac{\partial T}{\partial t} = -\sum_{i=1}^{n_s} \frac{\Delta h_{f,i}^0 \omega_i}{\rho c_p} \]

Consider single overall reaction

\[ CH_4 + OH \xrightarrow{k} CH_3 + H_2O \]

\[ k = A T^b \exp(-E / RT) \]

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

\[ A = 1.6 \cdot 10^7 \text{ (cm, mol, s)}, \quad b = 1.83, \quad E = 11.6 \text{ (kJ/mol)} \]
**HCCI:** Ignition delay

\[ \frac{\partial Y_i}{\partial t} = \frac{\omega_i}{\rho} \]

\[ \frac{\partial T}{\partial t} = -\sum_{i=1}^{n_s} \frac{\Delta h_{f,i}^0 \omega_i}{\rho c_p} \]

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 \( U \to U_0: \)

\[ m\beta t = \frac{1}{U_0^m} - \frac{1}{U^m} \]

So, time to reach, say, \( 5U_0: \)

\[ \beta t = \frac{4}{5mU_0^m} \]

**Cold boundary difficulty**

**Ignition delay**

\[ m\beta t = \text{Const.} - \frac{1}{U^m} \quad F_1(-m, m; (1 - m); U) \]
Hydrocarbon kinetics - NTC

Second Stage Ignition

\[ \text{H}_2\text{O}_2 = \text{OH} + \text{OH} \]

Acceleration by Q•OOH branching

Deceleration by olefin channel

First Stage Ignition

Isomerization steps

Hour 4: Engine combustion physics and chemistry

Warnatz, 2006

Hydrocarbon kinetics - NTC
HCCI combustion kinetics

Typical HCCI Combustion Temperature and Heat Release Rate profiles

R

H

- RH

+ O₂

+ O₂

. OOH

+ O₂

. OOH

. OO

- OH

HOO

Fast High Temperature Combustion

H₂O₂

Ethers/olefins

Degenerate Branching Path

Aldehydes/ketones

Mehl, 2009

Hour 4: Engine combustion physics and chemistry
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)
ERC-MultiChem: Primary Reference Fuel (PRF)

41 species, 158 reactions \(\rightarrow\) 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

<table>
<thead>
<tr>
<th>Physical property surrogates</th>
<th>Chemistry surrogates</th>
<th>LLNL Detailed mechanism</th>
<th>ERC reduced mechanism*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclo alkanes</td>
<td>cyclohexane</td>
<td>cyclohexane</td>
<td>1181 species 4269 reactions</td>
</tr>
<tr>
<td>n-alkane</td>
<td>n-heptane</td>
<td>n-heptane</td>
<td>570 species 2580 reactions</td>
</tr>
<tr>
<td>n-alkane</td>
<td>n-tetradecane</td>
<td>n-tetradecane</td>
<td>1168 species 6449 reactions</td>
</tr>
<tr>
<td>Iso-alkanes</td>
<td>iso-octane</td>
<td>iso-octane</td>
<td>857 species 3586 reactions</td>
</tr>
<tr>
<td>Aromatics</td>
<td>toluene</td>
<td>toluene</td>
<td>148 species 1036 reactions</td>
</tr>
</tbody>
</table>

**Chemical species and reactions summary:**
- **MultiChem Mechanism:** 100 species, 348 reactions
- **LLNL Detailed mechanism:** 857 species, 3586 reactions
- **ERC reduced mechanism:** 25 species, 51 reactions
- **Physical property surrogates:** 51 reactions
- **Chemistry surrogates:** 2018 reactions
Ignition delay validations - “MultiChem”

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

**Gauthier CNF 2004**

- Propane
  - $\phi=1.0$
  - $P_{in}=30$ bar

**Fieweger CNF 1997**

- *n*Heptane
  - $\phi=1.0$
  - $P_{in}=40$ bar

**Experiment**

<table>
<thead>
<tr>
<th>Model</th>
<th>Exp. Fieweger et al. (1997)</th>
</tr>
</thead>
</table>

**Bounaceur IJCK 2005; Andrae CNF 2005**

- Toluene

- $\phi=1.0$

- $P_{in}=40$ bar

**Shen, Energy & Fuels, 2009**

- iC8H18
  - $\phi=1.0$
  - $P_{in}=40$ bar

Hour 4: Engine combustion physics and chemistry

Ra, 2011
3-Dimensional models

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

Energy
\[
\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho I \mathbf{u}) = -\nabla \cdot \mathbf{J} + \dot{Q}^c + \dot{Q}^s - p \nabla \cdot \mathbf{u} + \mathbf{\sigma} : \nabla \mathbf{u}
\]
3-D CFD: Improved solver numerics

Sparse analytical Jacobian formulation

Sparsity of hydrocarbon fuel mechanisms increases with size

\[ \frac{\partial Y_i}{\partial t} = \frac{\omega_i}{\rho} \]

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

All functions and equations are evaluated in matrix form

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

<table>
<thead>
<tr>
<th>( n_s )</th>
<th>Time per Evaluation [ms]</th>
</tr>
</thead>
<tbody>
<tr>
<td>47</td>
<td>62.7%</td>
</tr>
<tr>
<td>160</td>
<td>86.2%</td>
</tr>
<tr>
<td>2878</td>
<td>99.7%</td>
</tr>
</tbody>
</table>

SpeedCHEM performance scaling

\[ \propto n_s \]

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 $\phi$)

$$\phi = \frac{2C_{-CO_2}^# + H_{-H_2O}^#/2 - z^rC_{-CO_2}^#}{O_{-CO_2-H_2O}^# - z^rC_{-CO_2}^#}$$
HCCI engine validation

ERC PRF mech. (39 sp, 141 rxn)

<table>
<thead>
<tr>
<th></th>
<th>Full</th>
<th>AMC</th>
<th>AMC+EDAC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>48.27 hrs.</td>
<td>3.99 hrs.</td>
<td>2.88 hrs.</td>
</tr>
</tbody>
</table>

Shi, 2012
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
Future emissions standards will be a challenging constraint.

Graph: 
- HC + NOx (gm/mile) vs. Year
- Data points for 7 Mode FTP, 80 Mode FTP (Clean Air Act), C/H 110 Mode FTP, TLEV, LEV, ULEV, LEV III (0.03 Forecast)
- Exponential curve showing reduction over time
- ~99.8% Reduction
NOx modeling

Zeldo’vich thermal NOx mechanism

\[ O + N_2 \leftrightarrow NO + N \quad \text{Rate controlling step due to high N}_2\text{ bond strength} \]

\[ N + O_2 \leftrightarrow NO + O \]

\[ N + OH \leftrightarrow NO + H \]

ERC 12-step NOx model is based on GRI-Mech v3.11 and includes:
- Thermal NOx \(^{\text{Zeldovich, 1946}}\)
- Prompt NOx around 1000 K. \(^{\text{Fenimore, 1979}}\)

Extensions
- NO can convert HCN and NH\(_3\) \(^{\text{Eberius, 1987}}\)
- Interaction between NO and Soot \(^{\text{Guo, 2007}}\)
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](http://www.erc.wisc.edu/combustion.php)


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


2-4:8 Curtis, E., Private communication, 2014


References


References


