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
Overview of optimization techniques

- Enumerative or exhaustive
- Calculus or gradient-based
  - “local” methods which search in the neighborhood of current design point
- Random
  - “global” methods such as genetic algorithms (GA) which typically converge on a global optimum
- Univariate (one-factor-at-a-time)
- Design of Experiments (DOE)
  - Two-level factorial designs (main and interaction effects)
  - Response surface methods (RSM)
  - Statistical model building
Genetic algorithms

“Individuals” are generated through random selection and a “population” is produced.

A model is used to evaluate the fitness of each individual.

The fittest individuals are allowed to “reproduce”.

A new “generation” is formed - “mutations” are allowed through random changes.

The fitness criteria thins out the population and the most fit solution is achieved over successive generations.
Implementation of algorithm

Binary representation of parameters $X$ - “genes”

$$X_1 \quad X_2 \quad X_3$$

10101101 01101 01001001

- “chromosome” gene string

Precision

$$\pi = \frac{X_{i,\text{max}} - X_{i,\text{min}}}{2^\lambda - 1}$$

Evaluate merit $f(X)$ for each generation member - identify “fittest” members

Binary tournament selection  Bit-swapping “Cross-over”

Parent 1

10101101 0110101001001 01100100 1110110101011

Parent 2

01100100 1110110101011

Descendants

10101101 1110110101011

01100100 0110101001001

10101101 1110110101011

01100100 0110101001001

Goldberg, 1989
Carrol, 1996
Senecal, 2000
**Optimization methodology**

**Multi-Objective Genetic Algorithm**

- Simultaneous optimization of many objectives [1]
- No merit function required to drive search
- Pareto front offers more information than a single optimum

**Nonparametric Regression Technique**

- Regression technique suitable for handling irregular and undesigned data sets (e.g., GA data) [2]
- Utilizes otherwise discarded optimization data
- Captures magnitude of effects AND the shape of their response

Liu, 2006
Coello, 2001
Example optimization - piston bowl design

Parameters and Objectives

Optimize:
- NOx
- Soot
- ISFC

7 Geometry Parameters:
- Pip height
- Bowl diameter
- $\phi$ of bowl bottom
- 4 curvature control points

Injector Spray Angle

Swirl Ratio
Pareto front designs

Bowl geometry or injection targeting trends?

- NOx ↓68%
- Soot ↑77%
- GISFC ↑15% (swirl = 0.7)

- NOx ↓57%
- Soot ↑6%
- GISFC ↓0% (swirl = 1.4)

- NOx ↓45%
- Soot ↓30%
- GISFC ↓2% (swirl = 3.1)

- NOx ↓5%
- Soot ↓42%
- GISFC ↓6% (swirl = 3.1)

Genzale, 2007

Hour 9: Optimization and Low Temperature Combustion
Regression – Identify dominant design parameters
Regression fits performed for each design on the Pareto front

- 3 dominant design parameters identified:
  1. Spray angle
  2. Swirl ratio
  3. Bowl diameter

Genzale, 2007
Regression – Understand Parameter Effects

**Response Surface Observations:**
An optimal spray angle is predicted.

Increased swirl ratio is predicted to enhance soot reduction near the optimal spray angle.

- Increases soot emissions at narrow spray angles.
- Increased swirl ratio is predicted to decrease soot at all bowl diameters.
Optimization of LTC - low temperature combustion

Increased interest in advanced combustion regimes

RCCI, HCCI, PCCI, MK - offer simultaneous reduction of NOx and soot

Challenges

High CO, HC
High loads
Transients

NOx
EGR
Soot
Combustion optimization - fuel and EGR selection

HCCI simulations used to choose optimal EGR rate and PRF (isooctane/n-heptane) blend

At 6, 9, and 11 bar IMEP 1300 rev/min

As load is increased the minimum ISFC cannot be achieved with either neat diesel fuel or neat gasoline

Predicted contours are in good agreement with HCCI experiments
**Charge preparation optimization**

Premixed and Direct Injected fuel blending

Desirable to use traditional diesel type injector
- Large nozzle hole (250 μm)
- Wide angle (145° included angle)

KIVA + Multi-Objective Genetic Algorithm (MOGA)

Fuel reactivity and EGR from HCCI investigation (9 bar IMEP)
- Global PRF = 65
- EGR rate = 50%

Five optimization parameters

Minimize two objectives
- Wall film amount
- PRF Inhomogeneity

Simulations run to 10 °BTDC

21 generations with a population size of 24

Kokjohn, 2009
Optimized Reactivity Controlled Compression Ignition (RCCI)

- Port injected gasoline
- Direct injected diesel
- Optimized fuel blending in-cylinder

Crank Angle (deg. ATDC)
- -80 to -50
- -45 to -30

Injection Signal

Kokjohn, 2009

PCI-3-9, 2018
### Heavy- and light-duty ERC experimental engines

<table>
<thead>
<tr>
<th>Engine</th>
<th>Heavy Duty</th>
<th>Light Duty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine</td>
<td>CAT SCOTE</td>
<td>GM 1.9 L</td>
</tr>
<tr>
<td>Displ. (L/cyl)</td>
<td>2.44</td>
<td>0.477</td>
</tr>
<tr>
<td>Bore (cm)</td>
<td>13.72</td>
<td>8.2</td>
</tr>
<tr>
<td>Stroke (cm)</td>
<td>16.51</td>
<td>9.04</td>
</tr>
<tr>
<td>Squish (cm)</td>
<td>0.157</td>
<td>0.133</td>
</tr>
<tr>
<td>CR</td>
<td>16.1:1</td>
<td>15.2:1</td>
</tr>
<tr>
<td>Swirl ratio</td>
<td>0.7</td>
<td>2.2</td>
</tr>
<tr>
<td>IVC (° ATDC)</td>
<td>-85 and -143</td>
<td>-132</td>
</tr>
<tr>
<td>EVO(° ATDC)</td>
<td>130</td>
<td>112</td>
</tr>
<tr>
<td>Injector type</td>
<td>Common rail</td>
<td></td>
</tr>
<tr>
<td>Nozzle holes</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>Hole size (µm)</td>
<td>250</td>
<td>128</td>
</tr>
</tbody>
</table>

Engine size scaling:
Staples, 2009
**Experimental validation** - HD Caterpillar SCOTE

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEP (bar)</td>
<td>9</td>
</tr>
<tr>
<td>Speed (rpm)</td>
<td>1300</td>
</tr>
<tr>
<td>EGR (%)</td>
<td>43</td>
</tr>
<tr>
<td>Equivalence ratio (-)</td>
<td>0.5</td>
</tr>
<tr>
<td>Intake Temp. (° C)</td>
<td>32</td>
</tr>
<tr>
<td>Intake pressure (bar)</td>
<td>1.74</td>
</tr>
<tr>
<td>Gasoline (% mass)</td>
<td>76, 82, 89</td>
</tr>
<tr>
<td>Diesel inject press. (bar)</td>
<td>800</td>
</tr>
<tr>
<td>SOI1 (° ATDC)</td>
<td>-58</td>
</tr>
<tr>
<td>SOI2 (° ATDC)</td>
<td>-37</td>
</tr>
<tr>
<td>Fract. diesel in 1st pulse</td>
<td>0.62</td>
</tr>
<tr>
<td>IVC (°BTDC)/Comp ratio</td>
<td>143/16</td>
</tr>
</tbody>
</table>

Computer modeling predictions confirmed
Combustion timing and Pressure Rise Rate control with diesel/gasoline ratio
Dual-fuel can be used to extend load limits of either pure diesel or gasoline

Hanson, 2010

**Effect of gasoline percentage**

![Graph showing the effect of gasoline percentage on pressure and apparent heat release rate.](image-url)
RCCI – high efficiency, low emissions, fuel flexibility

Indicated efficiency of $58\pm1\%$ achieved with E85/diesel

Emissions met in-cylinder, without need for after-treatment

Considerable fuel flexibility, including ‘single’ fuel operation

Diesel can be replaced with $<0.5\%$ total cetane improver (2-EHN/DTBP) in gasoline - less additive than SCR DEF
Dual fuel RCCI combustion – controlled HCCI

Heat release occurs in 3 stages (SAE 2010-01-0345, 2012-01-0375)

Cool flame reactions result from diesel (n-heptane) injection

First energy release occurs where both fuels are mixed

Final energy release occurs where lower reactivity fuel is located

Changing fuel ratios changes relative magnitudes of stages

Fueling ratio provides “next cycle” CA50 transient control
Understanding RCCI combustion

Location B with dummy plug installed

Optical Cylinder Head

Location A with optics installed

common rail injector

Port Fuel Injector

fiber to FTIR

common rail fuel spray

Hour 9: Optimization and Low Temperature Combustion

Splitter, 2010
Understanding RCCI combustion

Experimental in-cylinder FTIR measurements of combustion process at two locations

Spectra shows different fuel species at locations A and B, a result of the reactivity gradient

Fuel decomposition and combustion products form at a slower rate at location B, extending combustion duration
Light-duty drive-cycle performance

Compare conventional diesel combustion (CDC) and Reactivity Controlled Compression Ignition (RCCI) combustion

Compare at same operating conditions (CR, boost, IMT, swirl..)

ERC KIVA-Chemkin Code

Reduced primary reference fuel used to model diesel and gasoline kinetics

Suite of improved ERC spray models

Diesel fuel injector specifications

<table>
<thead>
<tr>
<th>Type</th>
<th>Bosch common rail</th>
</tr>
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<tbody>
<tr>
<td>Actuation type</td>
<td>Solenoid</td>
</tr>
<tr>
<td>Included angle</td>
<td>155°</td>
</tr>
<tr>
<td>Number of holes</td>
<td>7</td>
</tr>
<tr>
<td>Hole size (µm)</td>
<td>141</td>
</tr>
</tbody>
</table>

Combustion Chamber Geometry

Distance from firedeck [mm]

Distance from Centerline [mm]

Engine specifications

<table>
<thead>
<tr>
<th>Base engine type</th>
<th>GM 1.9 L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (mm)</td>
<td>82</td>
</tr>
<tr>
<td>Stroke (mm)</td>
<td>90.4</td>
</tr>
<tr>
<td>Connecting rod length (mm)</td>
<td>145.5</td>
</tr>
<tr>
<td>Squish height (mm)</td>
<td>0.617</td>
</tr>
<tr>
<td>Displacement (L)</td>
<td>0.4774</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>16.7:1</td>
</tr>
<tr>
<td>Swirl ratio</td>
<td>1.5 to 3.2</td>
</tr>
<tr>
<td>IVC (°ATDC)</td>
<td>-132°</td>
</tr>
<tr>
<td>EVO (°ATDC)</td>
<td>112°</td>
</tr>
</tbody>
</table>
Comparison - RCCI vs. conventional diesel

Five operating points of Ad-hoc fuels working group
Tier 2 bin 5 NOx targets from Cooper, SAE 2006-01-1145
(assumes 3500lb Passenger Car)
Evaluate NOx / fuel efficiency tradeoff using SCR for CDC

Assumptions
- Diesel exhaust fluid (DEF) consumption is 1% per g/kW-hr
- NOx reduction
  Johnson, SAE 2011-01-0304
- No penalty for DPF regeneration
- UHC and CO only contribute to reduced work

<table>
<thead>
<tr>
<th>Mode</th>
<th>Speed (rpm)</th>
<th>IMEP (bar)</th>
<th>CDC Baseline NOx (g/kgf) *</th>
<th>NOx Target (g/kgf)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1500</td>
<td>2</td>
<td>1.3</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>1500</td>
<td>3.9</td>
<td>0.9</td>
<td>0.4</td>
</tr>
<tr>
<td>3</td>
<td>2000</td>
<td>3.3</td>
<td>1.1</td>
<td>0.3</td>
</tr>
<tr>
<td>4</td>
<td>2300</td>
<td>5.5</td>
<td>8.4</td>
<td>0.6</td>
</tr>
<tr>
<td>5</td>
<td>2600</td>
<td>9</td>
<td>17.2</td>
<td>1.2</td>
</tr>
</tbody>
</table>

* Baseline CDC Euro 4: Hanson, SAE 2012-01-0380

Kokjohn, 2013

Ad-hoc fuels working group
SAE 2001-01-0151

Size shows relative weighting
## Euro 4 operating conditions - conventional diesel

### CDC Operating Conditions *

<table>
<thead>
<tr>
<th>Mode</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEPg (bar)</td>
<td>2.3</td>
<td>3.9</td>
<td>3.3</td>
<td>5.5</td>
<td>9</td>
</tr>
<tr>
<td>Speed (rev/min)</td>
<td>1500</td>
<td>1500</td>
<td>2000</td>
<td>2300</td>
<td>2600</td>
</tr>
<tr>
<td>Total Fuel (mg/inj.)</td>
<td>5.6</td>
<td>9.5</td>
<td>8</td>
<td>13.3</td>
<td>20.9</td>
</tr>
<tr>
<td>Intake Temp. (deg. C)</td>
<td>60</td>
<td>60</td>
<td>70</td>
<td>67</td>
<td>64</td>
</tr>
<tr>
<td>Intake Press. (bar abs.)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.3</td>
<td>1.6</td>
</tr>
<tr>
<td>EGR Rate (%)</td>
<td>47</td>
<td>38</td>
<td>42</td>
<td>25</td>
<td>15</td>
</tr>
<tr>
<td>CR Inj. Pressure (bar)</td>
<td>330</td>
<td>400</td>
<td>500</td>
<td>780</td>
<td>1100</td>
</tr>
<tr>
<td>Pilot SOI advance (°CA)</td>
<td>7</td>
<td>7</td>
<td>11</td>
<td>15</td>
<td>18</td>
</tr>
<tr>
<td>Main SOI (° ATDC) (actual)</td>
<td>-0.9</td>
<td>0</td>
<td>0.1</td>
<td>0.5</td>
<td>-1.8</td>
</tr>
<tr>
<td>Percent of DI fuel in Pilot (%)</td>
<td>20</td>
<td>15</td>
<td>15</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>

* Baseline CDC Euro 4: Hanson, SAE 2012-01-0380

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**Model validation**

- **Mode 2**
- **Mode 3**
- **Mode 4**
- **Mode 5**

*Kokjohn, 2013*
Model validation (Euro 4)

Comparison at 5 Modes

Cycle average emissions and performance

Optimized CDC with SCR for Tier 2 Bin 5

Weighted average:

\[ E_{cycle} = \frac{\sum_{i=1}^{5} E_{mode} Weight_{mode}}{\sum_{i=1}^{5} Weight_{mode}} \]
Comparison of efficiency, NOx and PRR

Target NOx at Tier 2 Bin 5

RCCI meets NOx targets without DEF

DEF NOx after-treatment has small efficiency penalty at light-load (2 to 4 bar IMEP) and moderate EGR (~40%)

DEF penalty is larger above 5 bar IMEP where EGR is below 40%

Kokjohn, 2013

Hour 9: Optimization and Low Temperature Combustion
RCCI and CDC compared at baseline and Tier 2 Bin 5 NOx
CDC NOx-GIE tradeoff controlled by main injection timing
RCCI meets NOx targets without after-treatment
RCCI gives ~8% improvement in fuel consumption over CDC+SCR
RCCI soot is an order of magnitude lower than CDC+SCR
RCCI HC is ~5 times higher than CDC+SCR
Currently addressing methods to reduce HC emissions
Crevice-originated HC emissions
Thermal barrier coated piston

Kokjohn, 2013

Cycle averaged NOx, Soot and GIE

![Bar chart showing NOx, Soot and GIE comparison between RCCI and CDC+SCR]
Limits of dual-fuel RCCI efficiency?

- Calibrate 0-D code with CR=14.88 experiments
- Use code to determine conditions needed to reach ~60% GTE

Results:

- ~60% GTE possible with:
  - High Cr
  - Lean operation (Φ<0.3)
  - 50% reduction in heat transfer & combustion losses

- Deactivate under-piston oil jet cooling

<table>
<thead>
<tr>
<th></th>
<th>Exp.</th>
<th>GT POWER</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression ratio</td>
<td>14.88</td>
<td>14.88</td>
</tr>
<tr>
<td>IMEPn (bar)</td>
<td>8.00</td>
<td>7.86</td>
</tr>
<tr>
<td>Fueling (mg/cyc)</td>
<td>87.13</td>
<td>87.13</td>
</tr>
<tr>
<td>Gross Therm Eff. (%)</td>
<td>54.3</td>
<td>54.5</td>
</tr>
<tr>
<td>Net Therm Eff. (%)</td>
<td>52.0</td>
<td>52.1</td>
</tr>
<tr>
<td>BTE (%)</td>
<td>45.3</td>
<td>45.1</td>
</tr>
<tr>
<td>FMEP (bar)</td>
<td>1.03</td>
<td>1.0</td>
</tr>
<tr>
<td>Convection HX</td>
<td>N/A</td>
<td>0.4</td>
</tr>
<tr>
<td>Comb. Eff. (%)</td>
<td>98</td>
<td>98</td>
</tr>
<tr>
<td>Intake Pressure (bar)</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>Exhaust Pressure (bar)</td>
<td>1.625</td>
<td>1.625</td>
</tr>
<tr>
<td>Turbo eff. (air filter + DOC)</td>
<td>67.5</td>
<td>62.3</td>
</tr>
</tbody>
</table>
High efficiency demonstrated!
Simulation heat transfer tuned to match data
14.88:1 required HX = 0.4
18.7:1 required HX = 0.3
(Pancake ~1.2 less surface area)
18.7:1 w/o oil cooling HX = 0.2

<table>
<thead>
<tr>
<th></th>
<th>GTE (%)</th>
<th>IMEPg (bar)</th>
<th>NTE (%)</th>
<th>IMEPn (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EXP (pt. 83)</td>
<td>59.1</td>
<td>6.82</td>
<td>55.0</td>
<td>6.27</td>
</tr>
<tr>
<td>GT Power HX =0.2</td>
<td>58.8</td>
<td>6.79</td>
<td>54.8</td>
<td>6.25</td>
</tr>
<tr>
<td>GT Power HX =0.4</td>
<td>56.7</td>
<td>6.55</td>
<td>52.8</td>
<td>6.02</td>
</tr>
</tbody>
</table>

94% of maximum theoretical cycle efficiency achieved!

Splitter, “RCCI Engine Operation Towards 60% Thermal Efficiency”, SAE 2013-01-0279
Hour 9: Optimization and Low Temperature Combustion

UW-Madison RCCI series hybrid vehicle

2009 Saturn Vue, V6 FWD base model → GM 1.9L diesel engine

SAE 2015-01-0837
Based on hot-start HWFET results, the vehicle is estimated to reach US EPA Tier2 bin5 NOx emissions with 53.5 mpg (4.4L/100km)

Installation of 7.5 gal. gasoline and diesel tanks

Spannbauer, 2014
Reitz, 2014,
Hanson, 2015, 2017
Closure

Availability of cheap energy has led to distorted world economies/priorities

7.2 Billion people: 1909 Haber-Bosch process making NH₃ for fertilizer

Next 30-40 years will require major innovations in IC engines
- dwindling resources and minimized environmental impact
- current energy usage rates are clearly unsustainable.

Many energy “solutions” (battery, fuel cell, nuclear) are only short term and resources are better saved for future generations

But, significant improvements in IC engines are still possible through research!

However, the only really long-term sustainable energy source is solar hydrogen. But, a switch to a H₂ economy will take considerable time and effort. Until this occurs, research on more efficient usage of fossil and other fuels is urgently needed!

“I’d put my money on the sun and solar energy. What a source of power! I hope we don’t have to wait until oil and coal run out before we tackle that.” Thomas Edison (1931) in conversation with Henry Ford and Harvey Firestone.
References


References


References


