Effect of the Composition of Hydrocarbon Streams on HCCI Performance

Rafal Gieleciak,^1 Craig Fairbridge,^1 Darcy Hager,^1 Bruce Bunting,^2 Thomas Gallant^3 and Ken Mitchell^4

^1 CanmetENERGY, ^2 Oak Ridge National Laboratory, ^3 Pacific Northwest National Laboratory, ^4 Shell Canada
Introduction

- Evolving fuels and combustion strategies have resulted in advanced combustion engines that may have varying fuel quality appetites when compared to conventional engines.
- At the same time, advanced analytical methods are becoming both more powerful and easier to use.
  - Two examples are NMR and 2D-GC (two dimensional gas chromatography).
- Statistical analysis allows us to link the very complex fuel analysis data sets from these methods to fuel chemistry and properties and to engine performance.
- Purpose of research covered in this presentation:
  - To apply an advanced statistical analysis technique to 2D-GC data for 17 oil sands derived fuels and correlate results to measured fuel chemical / physical properties, and then to HCCI engine performance.
Background

Goal – identify knowledge gaps in using future fuels from all sources in advanced engines

1. Chemical analysis
2. Highly efficient clean combustion
3. Relationship between 1 and 2 above
4. Standard light petroleum derived fuels
5. Standard oil sands derived fuels
6. Typical compounds for surrogate fuels
7. Combustion-based performance measure

HCCI engine

Homogeneous Charge Compression Ignition

In the HCCI mode ignition occurs due to compression of the homogeneous fuel/air mixture. It is a simple platform for fuels research.
Advanced combustion strategies must satisfy the need for high efficiency, low emissions, and driveability.
It is not obvious which fuel chemical or physical properties are responsible for processes occurring during advanced combustion.

- 17 refinery streams consisting of finished fuels and process streams were obtained from oil sands derived crude oil
- The samples were characterized for chemical and physical properties and run in a simple premixed HCCI engine
- The intent was to study as wide a range of oil sands related fuel chemistry and properties as possible and to relate this information to HCCI engine performance
- In HCCI combustion, the engine preferred lower cetane number fuels with lower boiling points

SAE paper 2008-01-2406
ORNL HCCI research engine

- Engine
- Intake Air Heater
- Belt Drive
- Atomizing Injector
- Constant Speed Motoring Dyno

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine Displacement (cc)</td>
<td>517</td>
</tr>
<tr>
<td>Bore (cm)</td>
<td>9.7</td>
</tr>
<tr>
<td>Stroke (cm)</td>
<td>7.0</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>10.5:1</td>
</tr>
<tr>
<td>Intake Valve Opening (CA deg)</td>
<td>710</td>
</tr>
<tr>
<td>Intake Valve Closing (CA deg)</td>
<td>218</td>
</tr>
<tr>
<td>Exhaust Valve Opening (CA deg)</td>
<td>499</td>
</tr>
<tr>
<td>Exhaust Valve Closing (CA deg)</td>
<td>20</td>
</tr>
<tr>
<td>Intake Air Temperature (°C)</td>
<td>30 - 400</td>
</tr>
</tbody>
</table>

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Two Dimensional Gas Chromatography

1st column
non-polar

2nd column
semi-polar

GC x GC Chromatograms generate separations in two dimensions - first dimension is primarily a “size” separation - second dimension is primarily a “polarity” separation

Figure 6-1
2 Stage Thermal Modulator

injector
detector
Two Dimensional Gas Chromatography

1D GC separation often suffer from coelutions for samples containing more than 150 compounds. 2D-GC provides a comprehensive two dimensional separation where the entire sample is separated on two different columns. Technology capable of separating hundreds to thousands more compounds in complex mixtures. One of the advantages of using 2D-GC for chromatographic separation is the high degree of organization based on chemical structure that can be seen in the resulting chromatogram.

- saturates
- Naphthenic monoaromatics
- monoaromatics
- Naphthenic di-aromatics
- di-aromatics
- tri-aromatics

RT2 [s]  3.58

RT1 [s]  1.58  1176  2176

C0  C1  C2  C3  C4
Quantitative Two-Dimensional Retention Property Relationship
Q(2d)RPR

2D-GC chromatograms are fingerprints of petrochemical samples. These profiles describe the composition of hydrocarbon samples and can be treated as compositional variables which could describe bulk properties of the samples.
Q(2d)RPR How it works?

**STEP 1: Data receiving**

- **HCCI Engine**
- **GCxGC-ToFMS**
- **IMEP ratio**
- **ISFC values**
- **SMOKE**
- **IntakeT**
- **NOx, HC, CO emission level**

**Dependent variables (properties)**

**“Independent” variables (predictors)**
**Q(2d)RPR** How it works?

**STEP 2: Q(2d)RPR Analysis**

- **CALIBRATION**
  - e.g. PLS
  - predict fuel properties

- **CLASSIFICATION**
  - e.g. PCA
  - fuels grouping

**feature extraction** (variable selection)
Q(2d)RPR How it works?

GCxGC chromatograms

Unfold chromatograms

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PLS (Projection to Latent Structures) regression is a generalization of multiple linear regression (MLR) but unlike MLR, it can analyze data with strong collinear (correlated), noisy, and numerous X-variables and model the relationship between X and Y.

The linear PLS model finds “new” variables, a latent variables (X-scores). These scores are linear combination of the original variables and they have following properties: they are good predictors of Y, they are few in number and they are orthogonal.

PLS is a projection method and, thus has a simple geometric interpretation with a projection of the X matrix (a swarm of points in N-dimensional space) on to an A-dimensional hyperplane in such a way that the coordinates of the projection are good predictors of Y)
**Samples characteristics**

- 17 samples (100%) derived from Canadian oil sands crude
- Half of the streams upgraded by coking and half by hydrocracking
- All streams are nominally of diesel boiling point range
- All had sulfur levels below 15 ppm (except one)
- All had diverse chemistry

**Physicochemical and Engine Properties**

*Cetane number, n-paraffins, iso-paraffins, mono-cycloparaffins, poly-cycloparaffins, mono-aromatics, poly-aromatics, Olefins, T10, T50, T90, density, viscosity, carbon, hydrogen*

*Smoke, HC (ppm), CO (ppm), NOx (ppm), COV (%), MFB50, CA10-90, dP/dCA, %LTHR, ISFC, ITE*
GCxGC chromatograms of HCCI fuels
Results of PLS Analysis

**Physicochemical**

- $q^{2}_{cv \, model}$ – correlation coefficient after cross-validation

The cross-validated correlation parameter ($q^{2}_{model}$) > 0.5 generally is regarded as good and a $q^{2}_{model}$ > 0.9 as excellent

\[
q^{2}_{cv \, model} = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y}_i)^2}
\]
Q(2d)RPR (CORRELATIONS)

MFB50 – crank angle position for 50% of the fuel to be burned, determined from heat release analysis

ISFC – indicated specific fuel consumption
Projection of coefficients of PLS equation

\[ b_1 x_1 + b_2 x_2 + \ldots + b_N x_N \]

The red color indicates positive contribution and blue color negative contribution.
Projection of coefficients of PLS equation
Conclusions

- 2D-GC is an emerging analytical technique which separates compounds in fuels. This allows analysis by
  - Identifying individual compounds
  - Grouping compounds by chemistry and boiling points
  - Performing statistical analysis by treating the chromatograms as compositional descriptors of fuels
- Q(2d)RPR technique allows correlations to be developed between the 2D-GC data and fuel chemical / physical properties and engine performance data (quantitative 2D retention property relationship)
  - Regions of chromatograms were shown to correlate, positively and negatively, to the values of fuel properties (cetane number, viscosity) and to HCCI research engine performance (MFB50, %LTHR)
  - This technique provided good correlations for some properties indicating that it is worthy of further study
Future work

• Continue to develop chemistry class and exact compound identification for 2D-GC
• Continue to develop and improve the statistical techniques that can be applied to large complex data sets
• Future work will include examining fuel-engine correlations with other selection criteria such as constant intake temperature or constant combustion phasing
• Improve engine model side of model by accounting for additional independent variables
• Apply technique to other performance related fuels data, such as lubricity or seal swell, and to performance from other types of engines
Acknowledgements

Program on Energy Research and Development, Natural Resources Canada

Vehicle Technologies Program, Energy Efficiency and Renewable Energy, Department of Energy