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Leadership in ecoInnovation

Effect of the Composition of Hydrocarbon Streams on HCCI Performance

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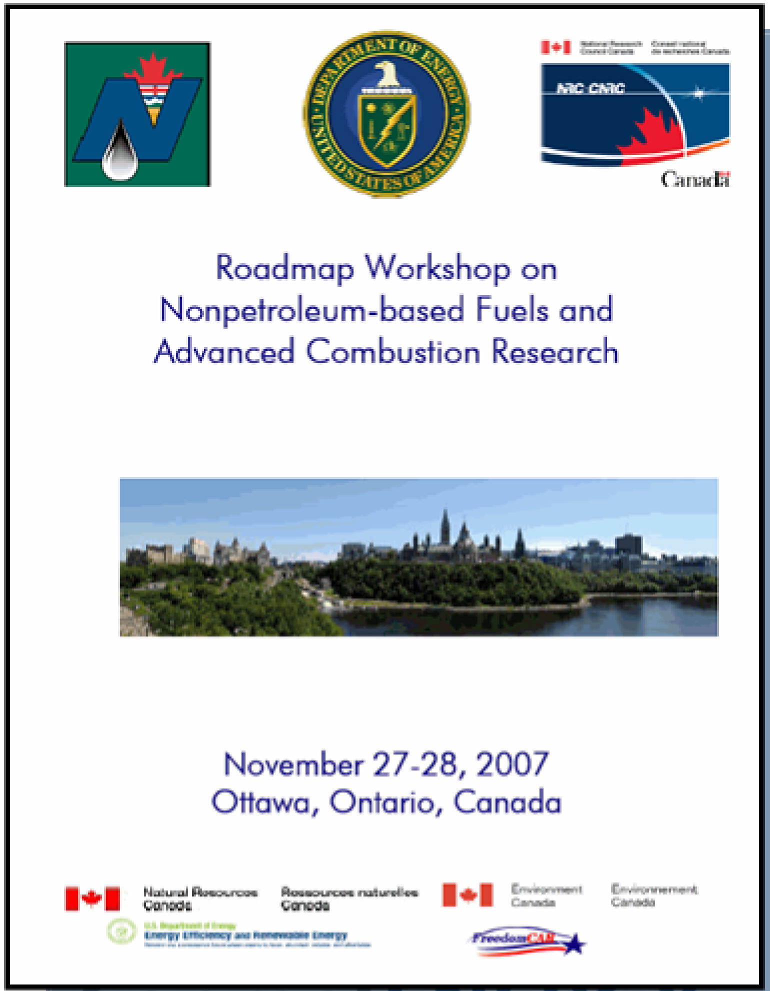
Introduction

- 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 allow 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

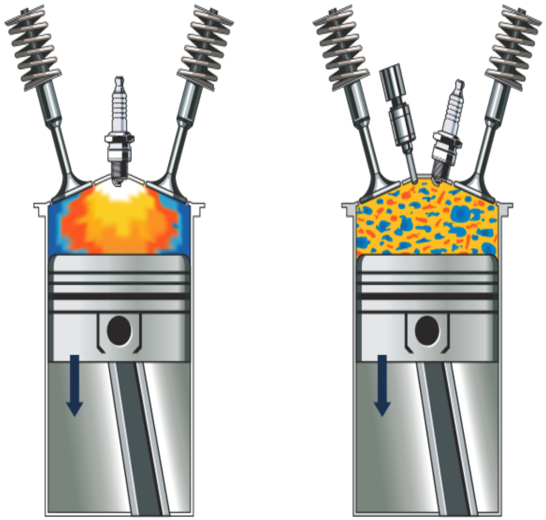
1. Chemical analysis
2. Highly efficient clean combustion
3. Relationship between 1 and 2 above
4. Standard light petroleum derived fuels
5. Standard oil sands derived fuels
6. Typical compounds for surrogate fuels
7. Combustion-based performance measure



http://canmetenergy-canmetenergie.nrcan-rncan.gc.ca/eng/oil_sands/future_fuels_emissions.html

HCCI engine

Homogeneous Charge Compression Ignition

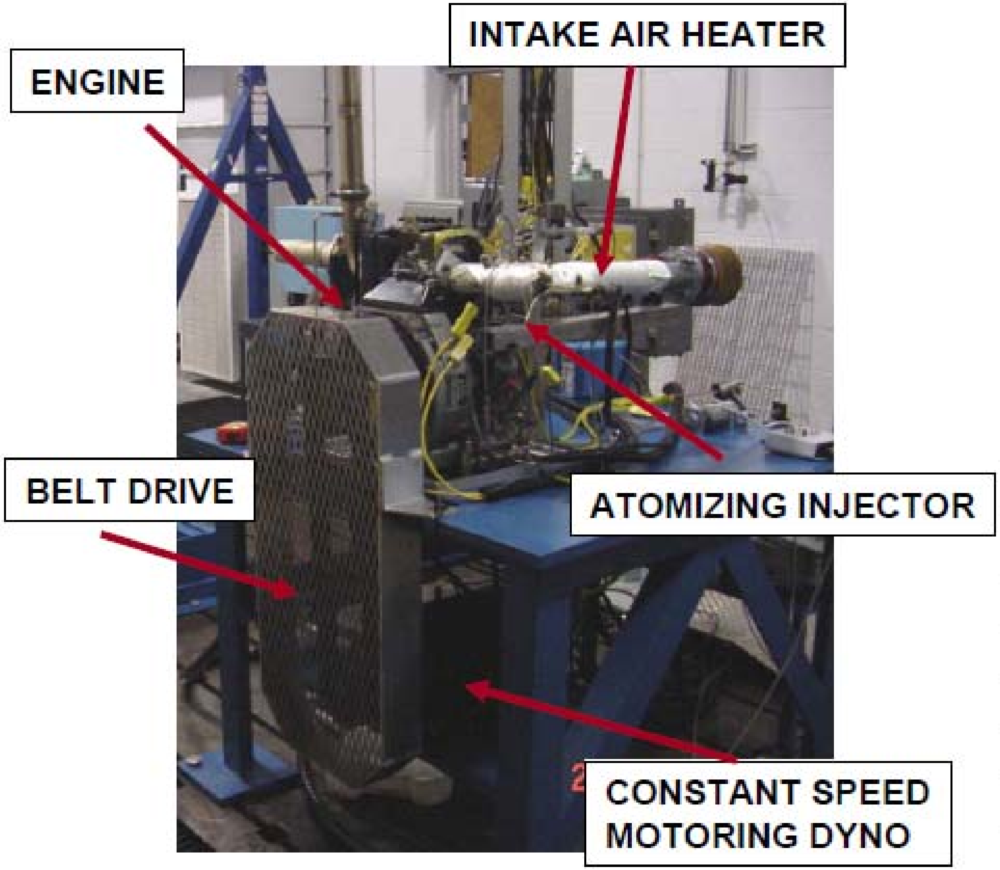


In the HCCI mode ignition occurs due to compression of the homogeneous fuel/air mixture. It is a simple platform for fuels research.
Advanced combustion strategies must satisfy the need for high efficiency, low emissions, and driveability.
It is not obvious which fuel chemical or physical properties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



MODIFIED PISTON
WITH SPHERICAL
COMBUSTION BOWL

Engine Displacement (cc)	517
Bore (cm)	9.7
Stroke (cm)	7.0
Compression Ratio	10.5:1
Intake Valve Opening (CA deg)	710
Intake Valve Closing (CA deg)	218
Exhaust Valve Opening (CA deg)	499
Exhaust Valve Closing (CA deg)	20
Intake Air Temperature (°C)	30 - 400

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Two Dimensional Gas Chromatography

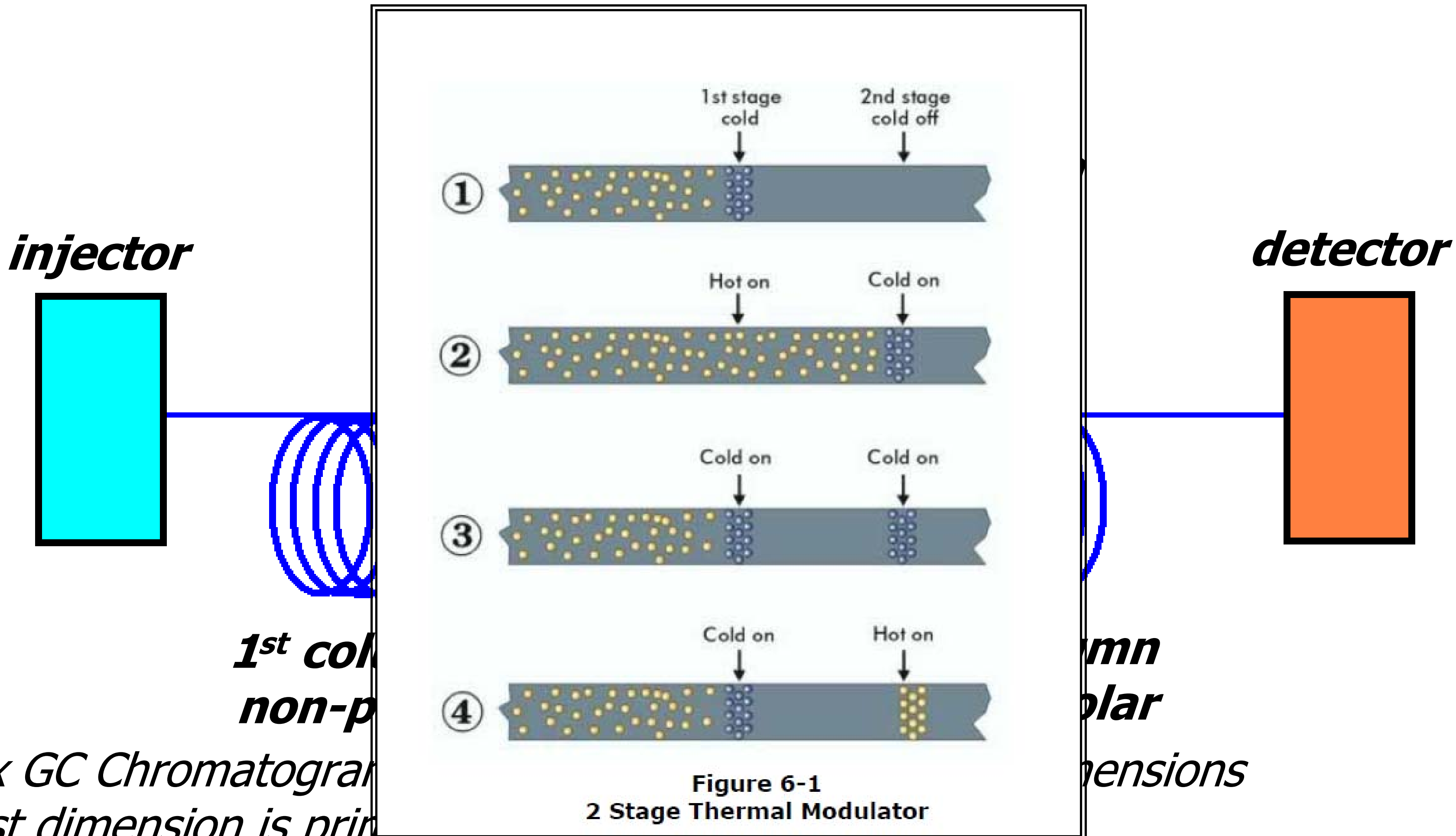
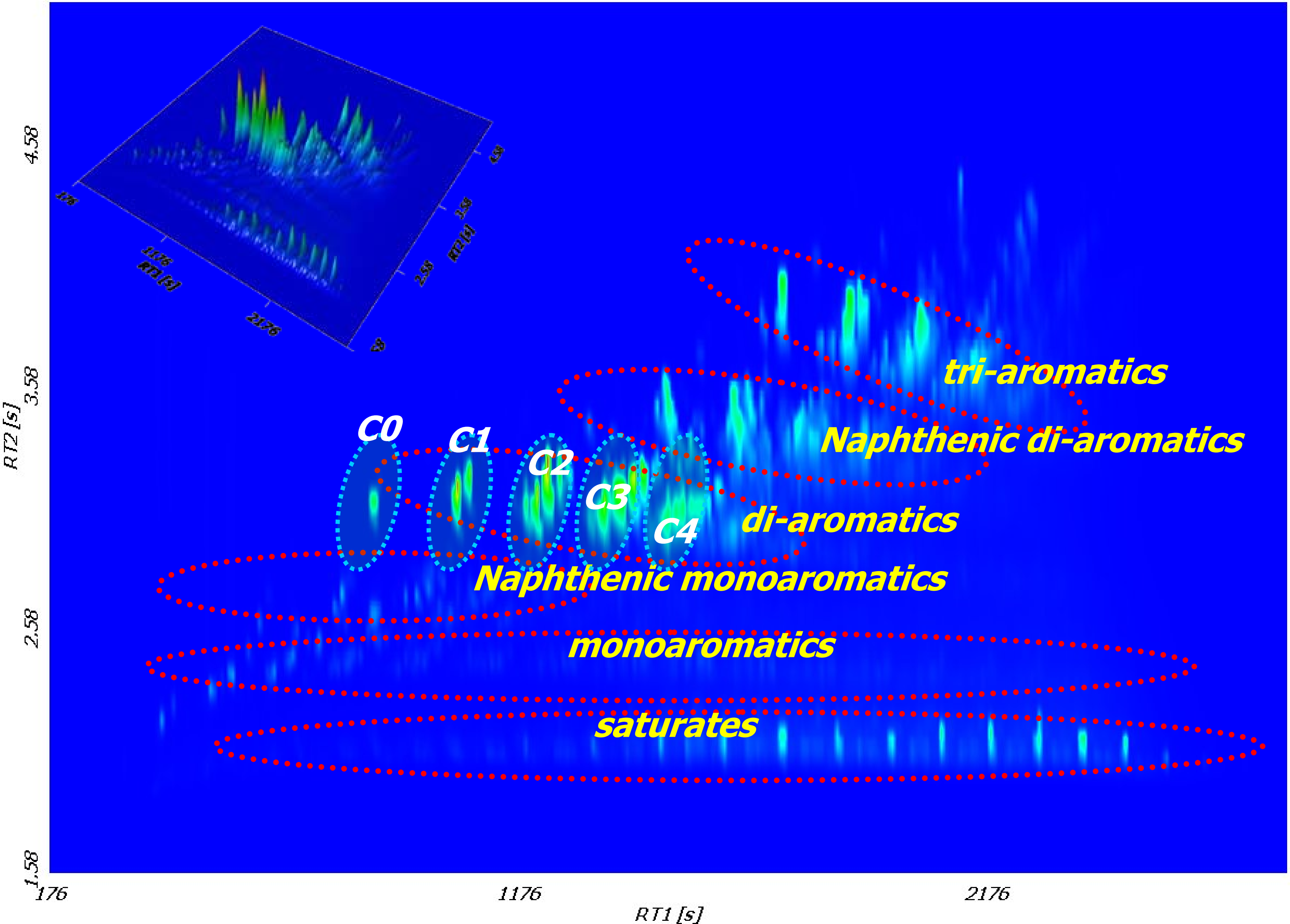


Figure 6-1
2 Stage Thermal Modulator

GC x GC Chromatogra ensions
- first dimension is pri
- second dimension is primarily a "polarity" separation

Two Dimensional Gas Chromatography

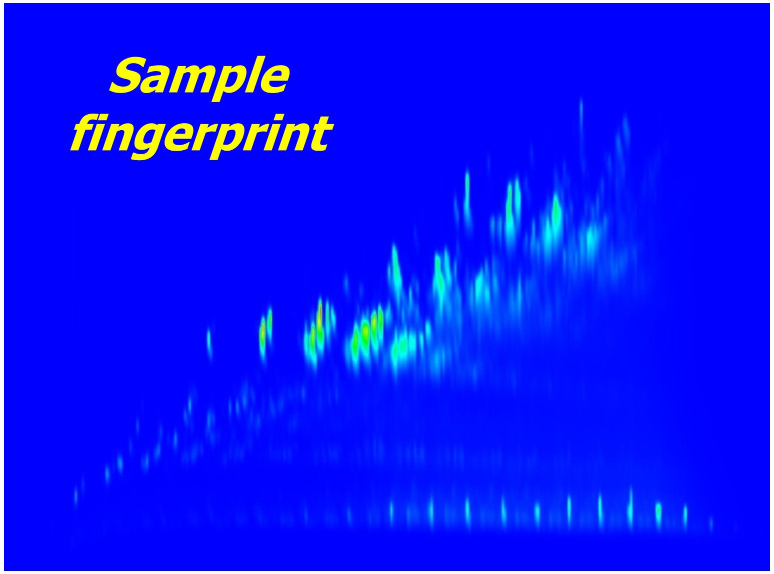


Q(2d)RPR

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



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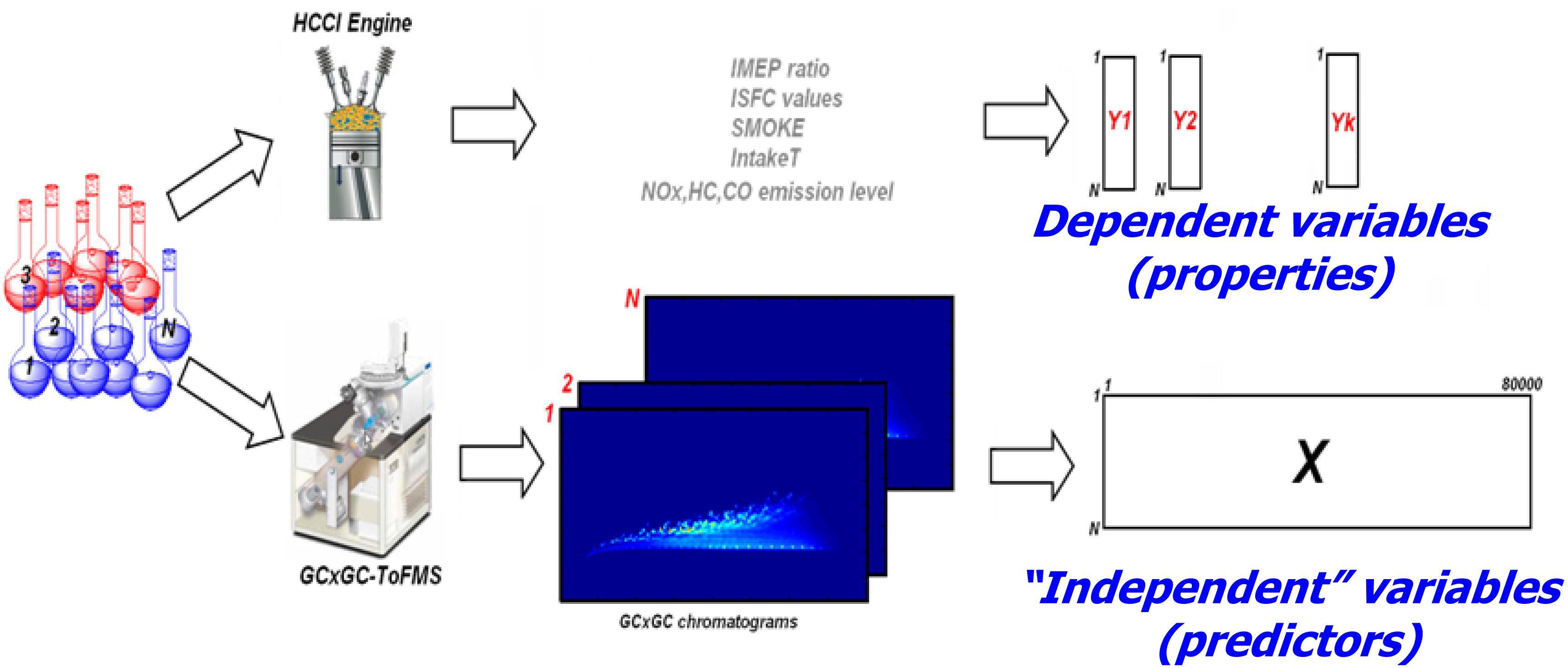
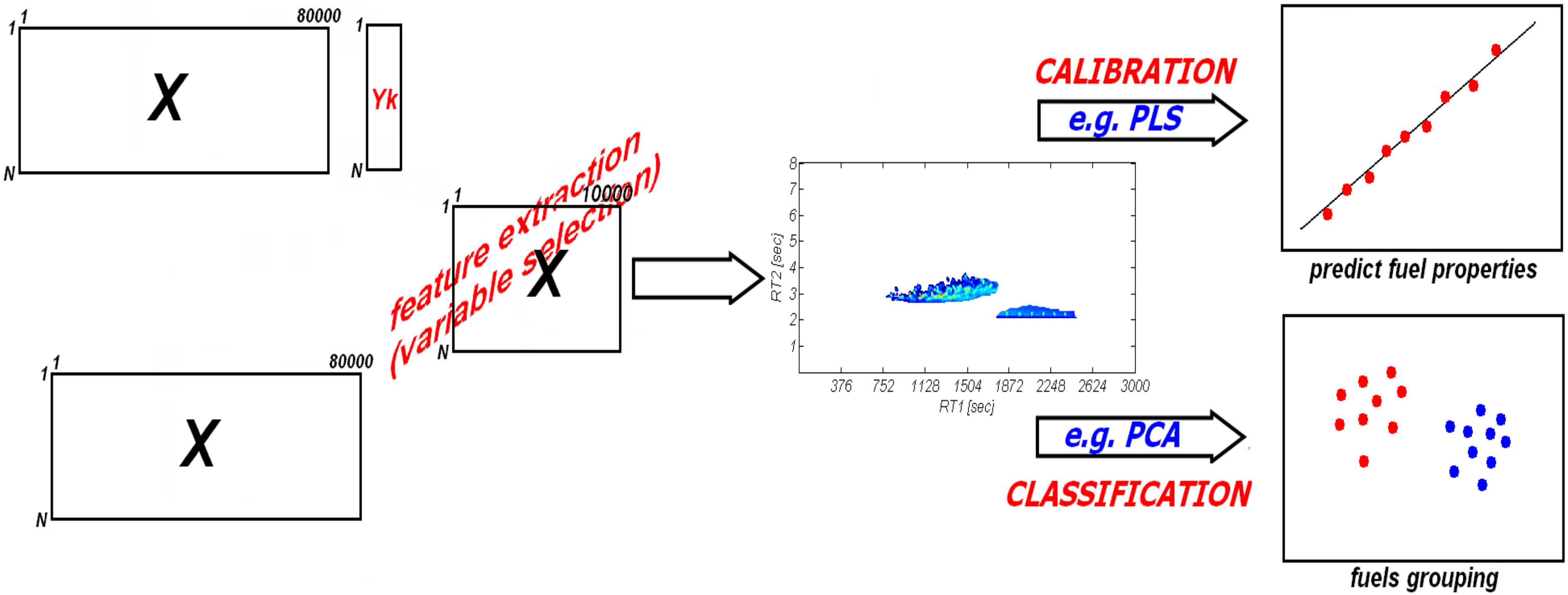
Q(2d)RPR How it works?

STEP 1: Data receiving

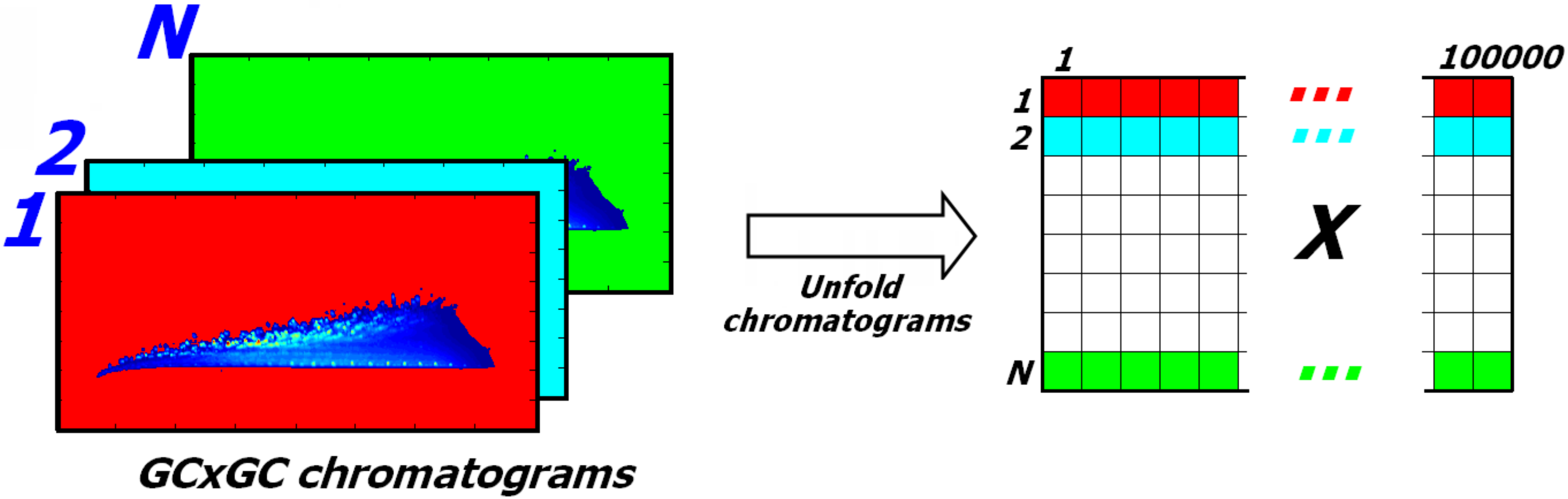


Q(2d)RPR How it works?

STEP 2: Q(2d)RPR Analysis



Q(2d)RPR How it works?

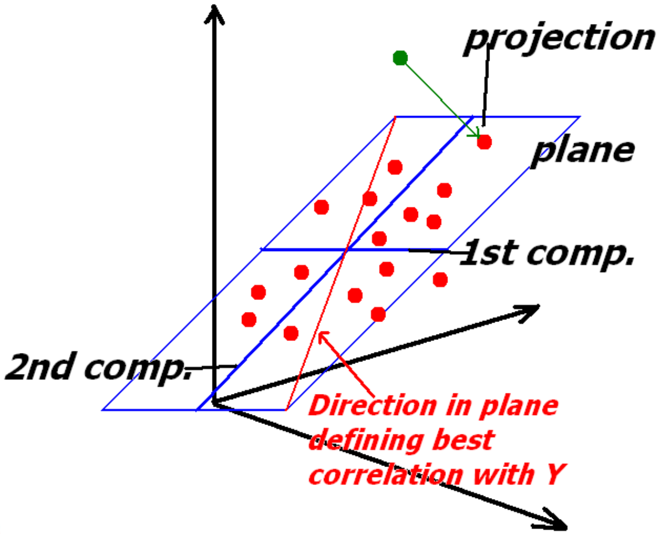


Projection to Latent Structures

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

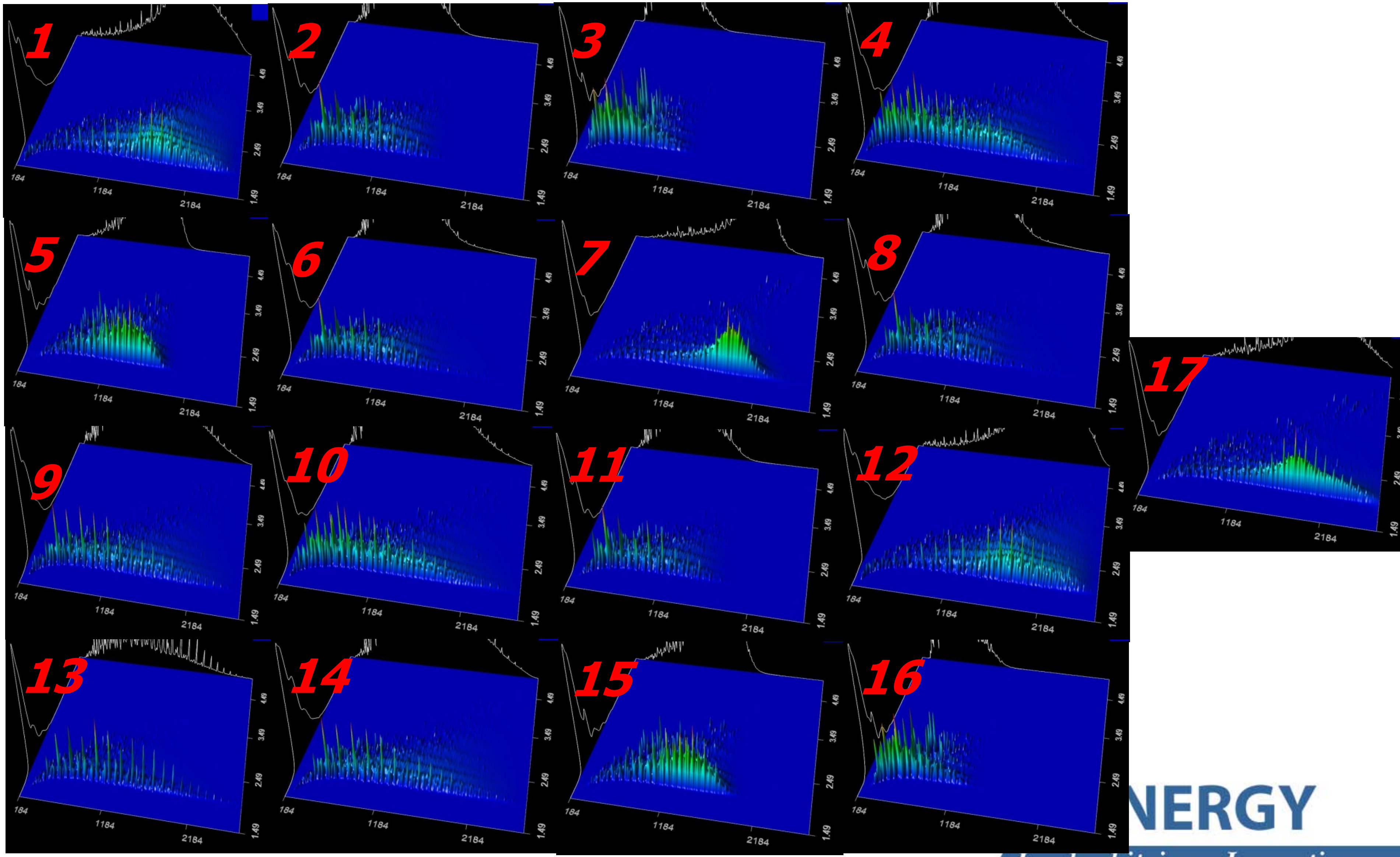
- 17 samples (100%) derived from Canadian oil sands crude
- Half of the streams upgraded by coking and half by hydrocracking
- All streams are nominally of diesel boiling point range
- All had sulfur levels below 15 ppm (except one)
- All had diverse chemistry

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

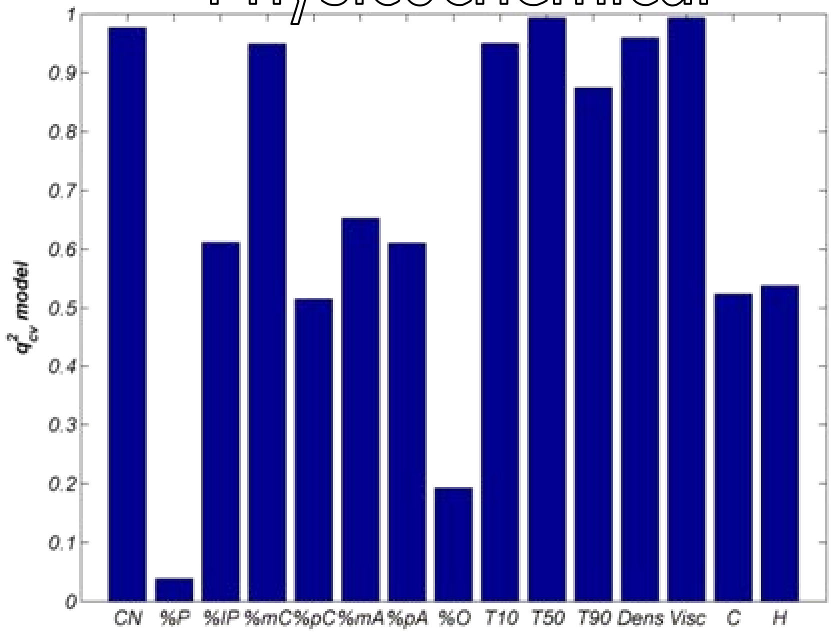
GCxGC chromatograms of HCCI fuels



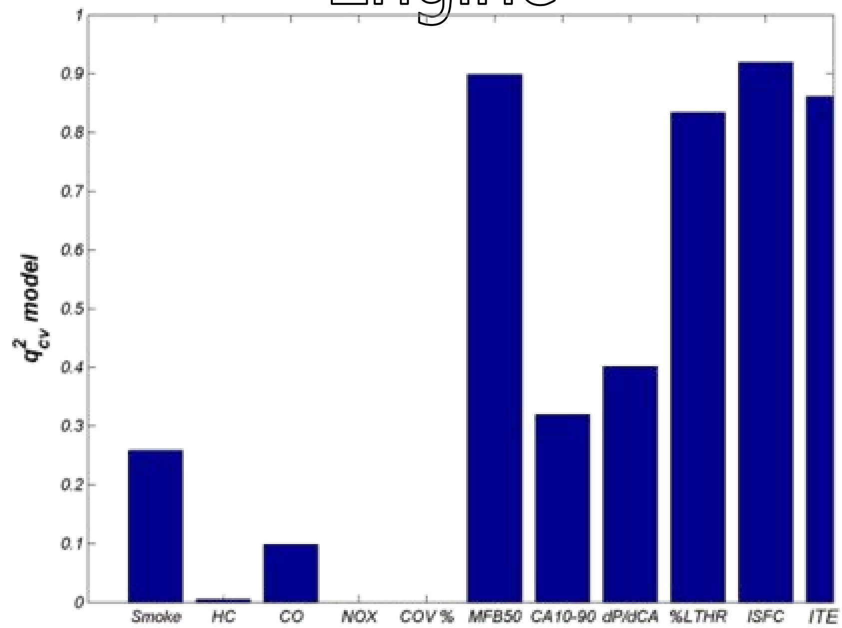
Q(2d)RPR

Results of PLS Analysis

Physicochemical



Engine

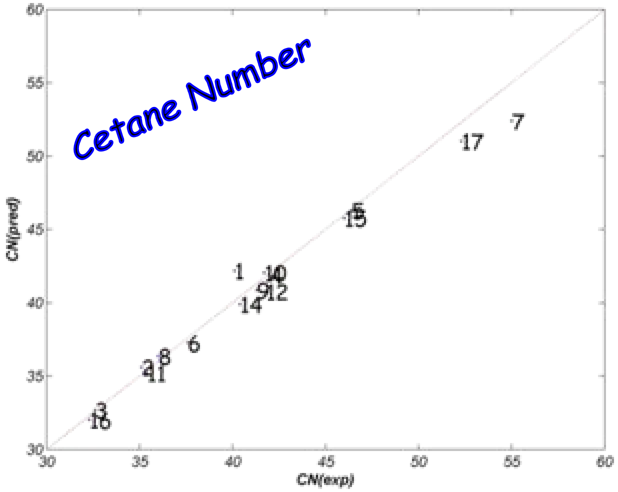


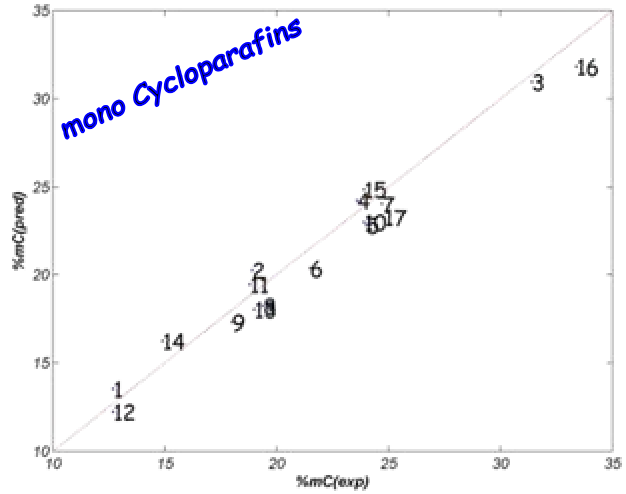
q^2_{cv}model – *correlation coefficient after cross-validation*

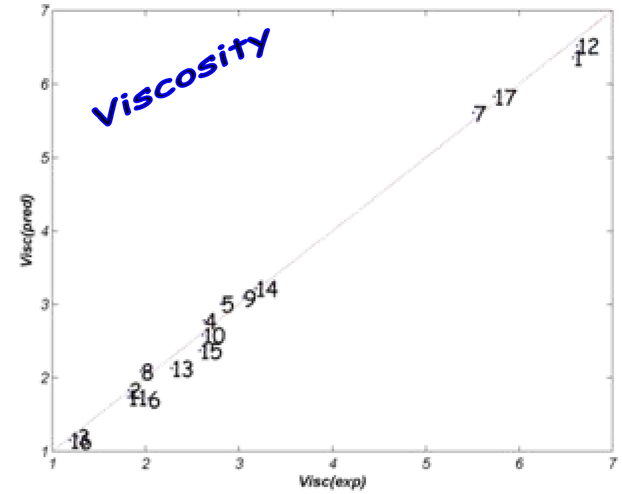
The cross-validated correlation parameter (q2model) > 0.5 generally is regarded as good and a q2model > 0.9 as excellent

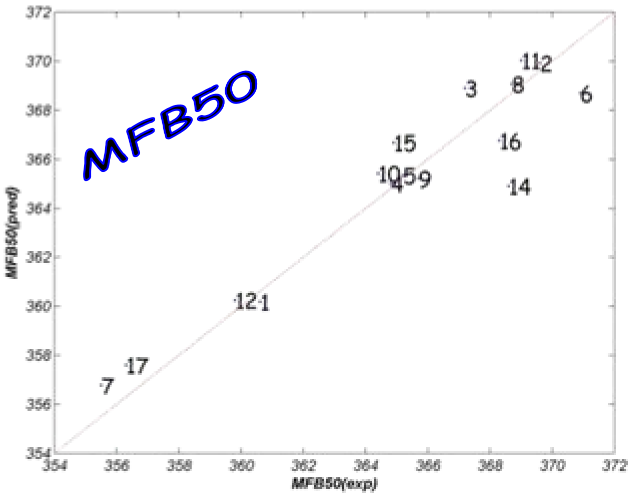
$$q^2{}_{cv}\,model = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y}_i)^2}$$

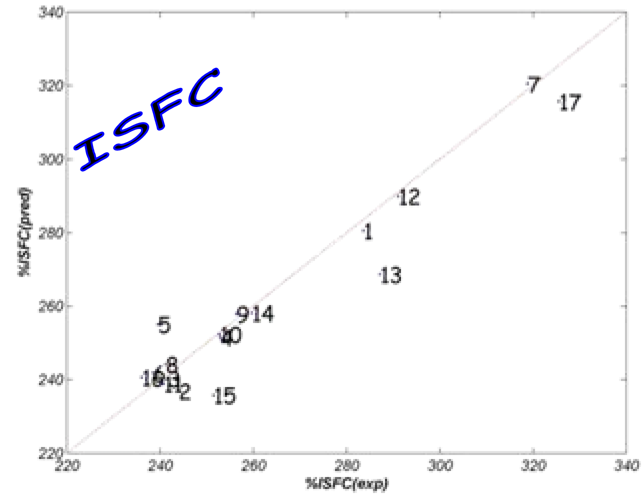
Q(2d)RPR *(CORRELATIONS)*











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

***ISFC** – indicated specific fuel consumption*

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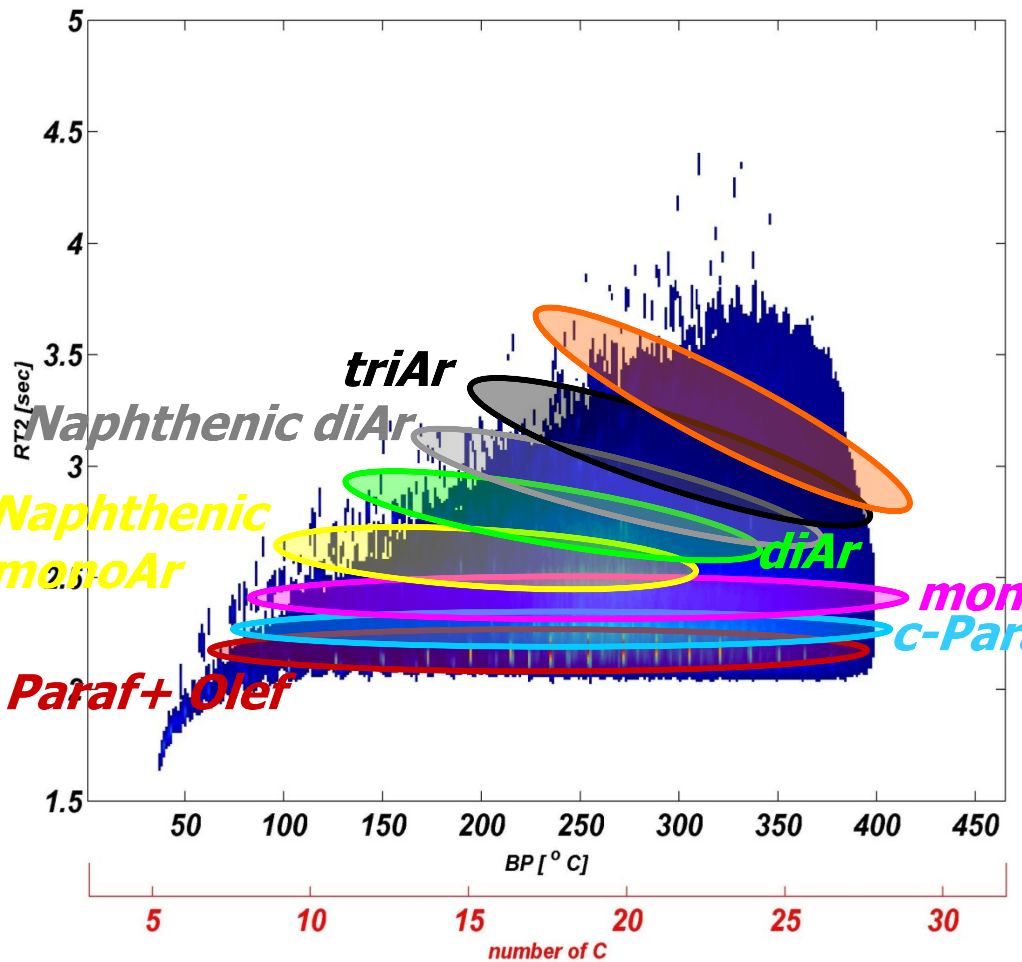
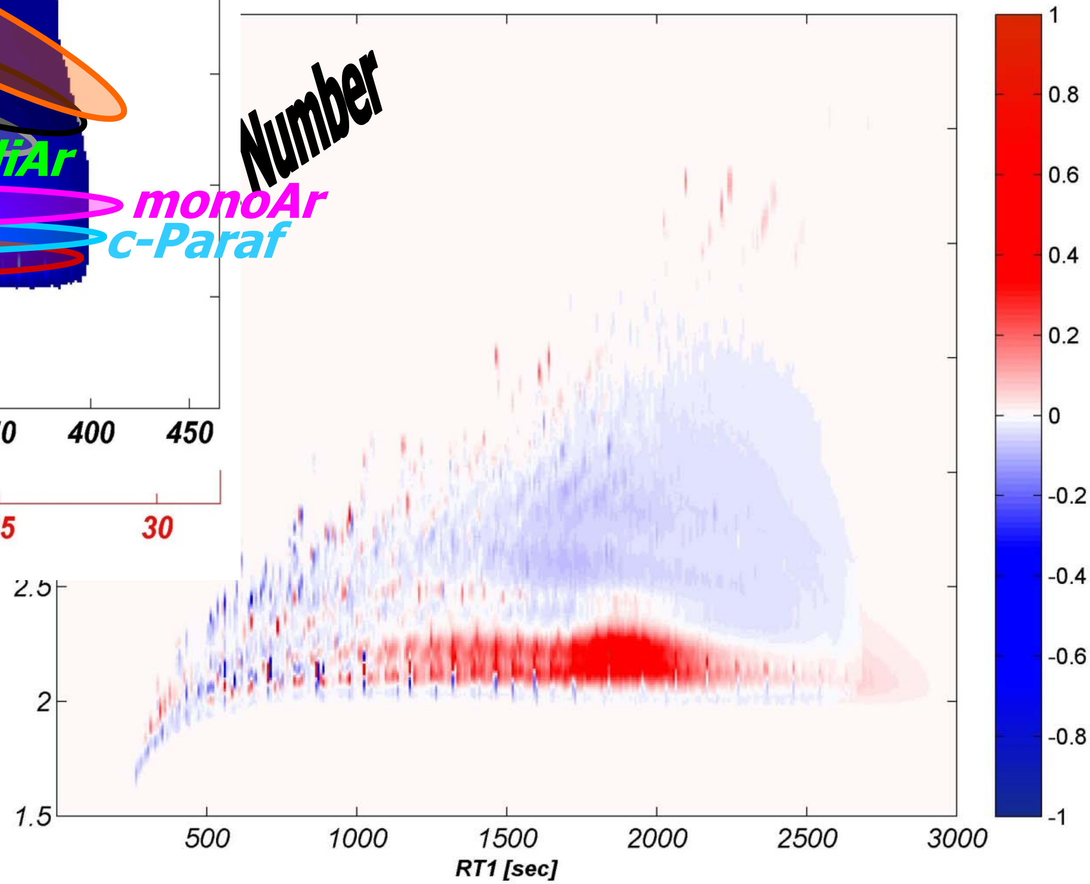
RPR

nts of PLS equation

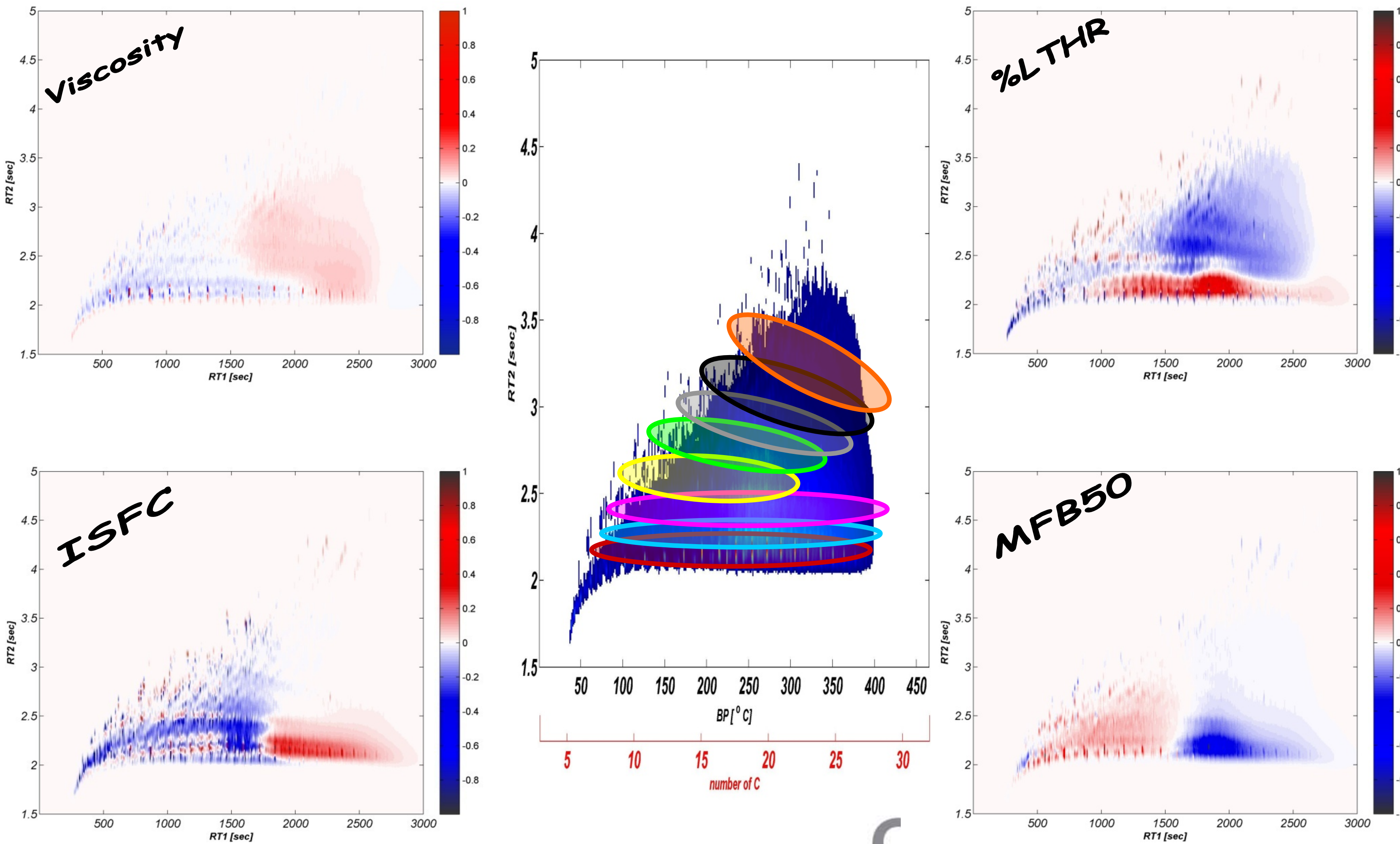
$$_3 x_3 + b_4 x_4 + \dots + b_N x_N$$





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

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