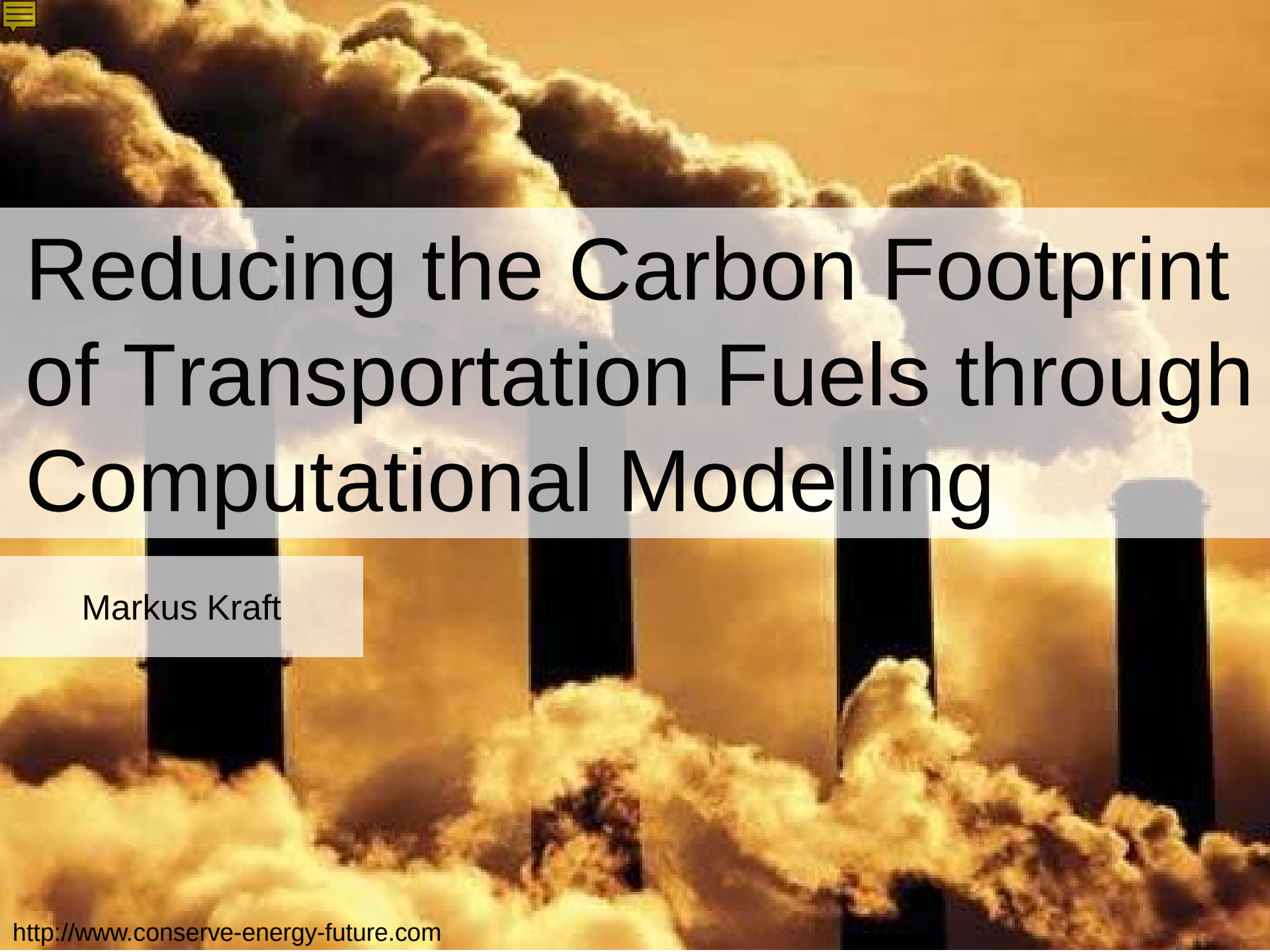
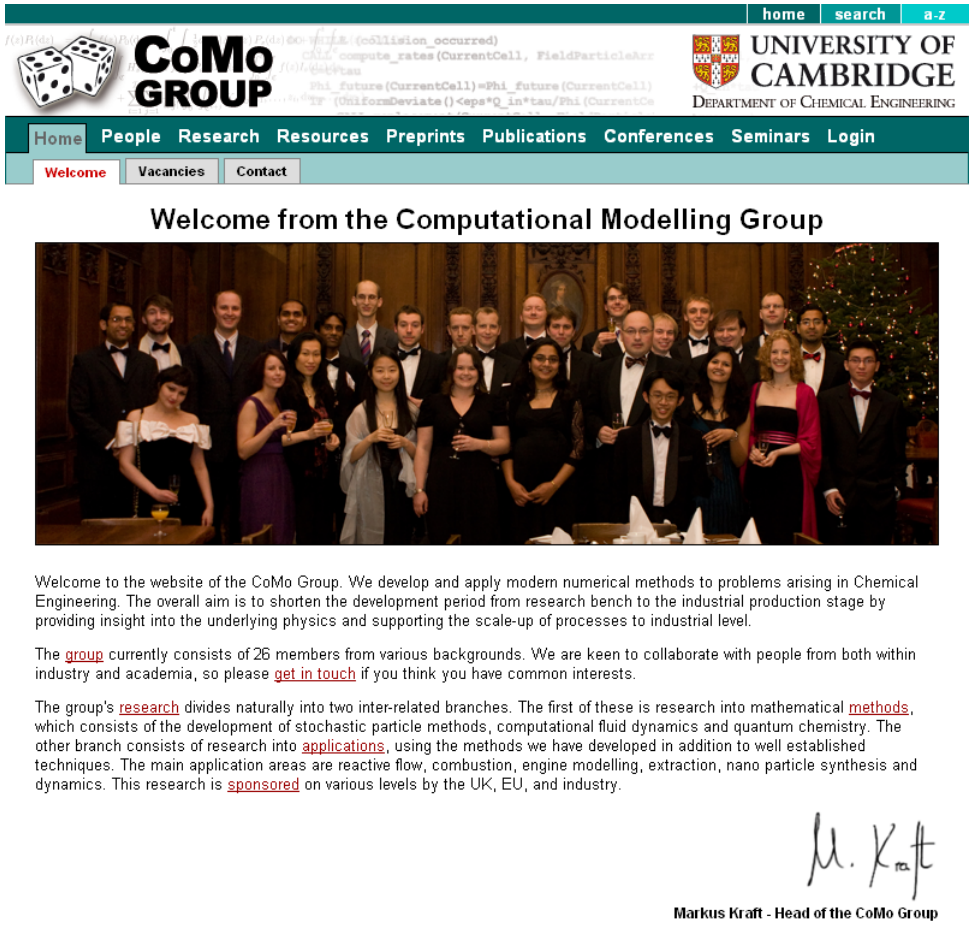


Reducing the Carbon Footprint of Transportation Fuels through Computational Modelling

Markus Kraft

Computational Modelling Group

- Founded in 1999
- Head **Prof. Markus Kraft**
- Currently 20 members (PhDs, PDRAs)
- Theme: Modelling across the length scales



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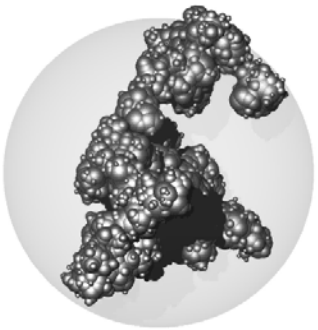
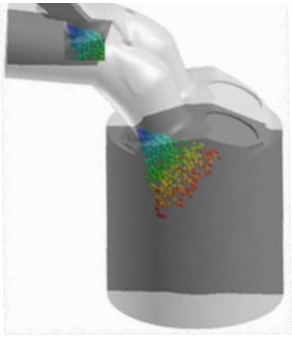
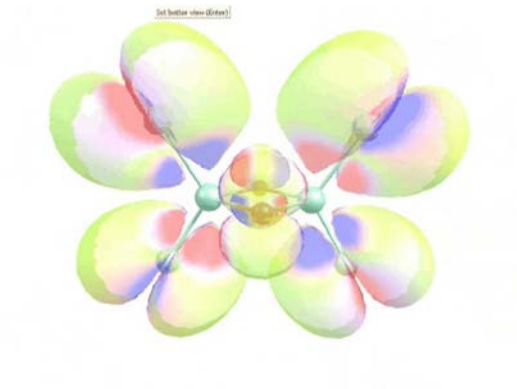
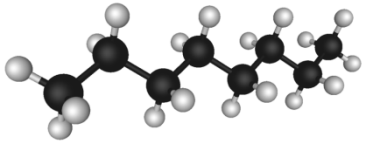
Emphasis: **Combustion**

- Particulate processes (**nanoparticles, soot**)
- **Emissions** from **Internal Combustion Engines**









Methods:

- Quantum chemistry
- Population balance modelling
- Computational Fluid Dynamics
- Process optimisation

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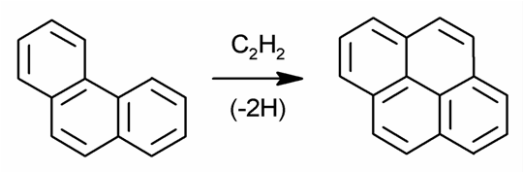
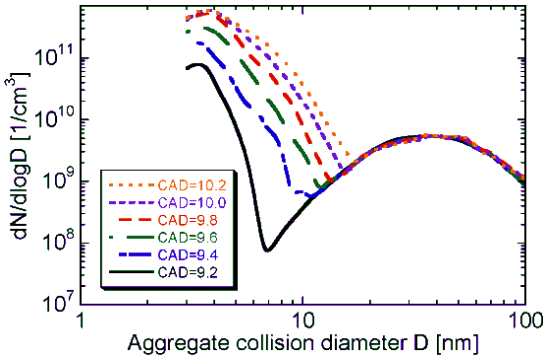
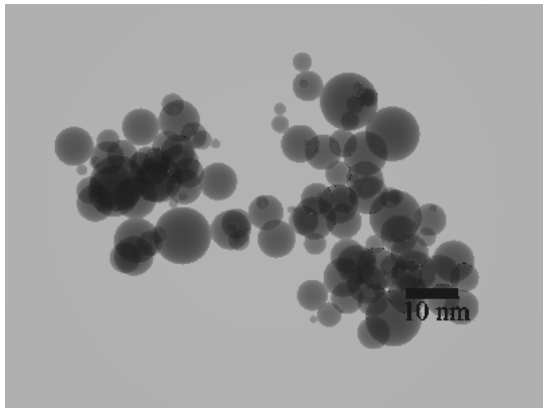


Emissions from internal combustion engines:

- Stochastic Reactor Model
- **CO, uHC, NOx, etc.** through **detailed chemical kinetics**
- **Soot** through **detailed population balance models**





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Process Informatics:

- Effective use of cost-intensive experimental data through **data standardisation**

- Robust model development through **systematic optimisation**, accounting for **uncertainties**

- **Design of experiments**

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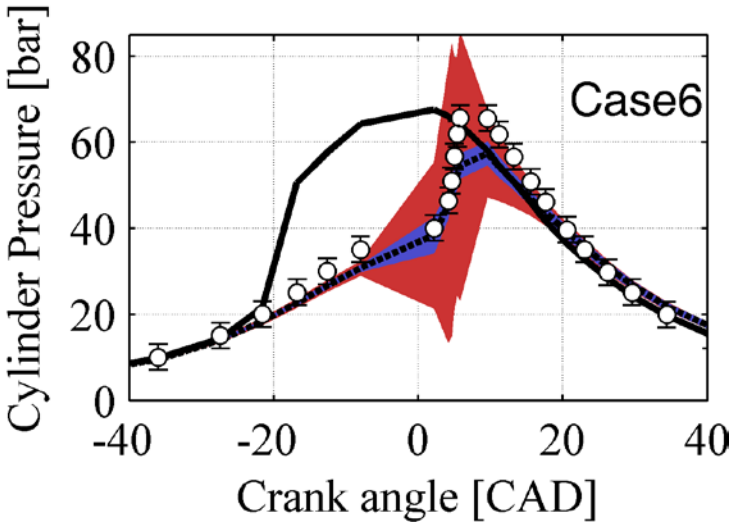

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Reducing CO_2

Reducing CO_2

Improve Low Carbon Feedstock Fuel Blends

Help Prevent Climate Change

Protect Human Health

Methodology Development

Automated Experiments

Automatic Model Building

Standardised Data

Model Development

Chemistry Flow Interaction

Reaction Kinetics

Particle Formation

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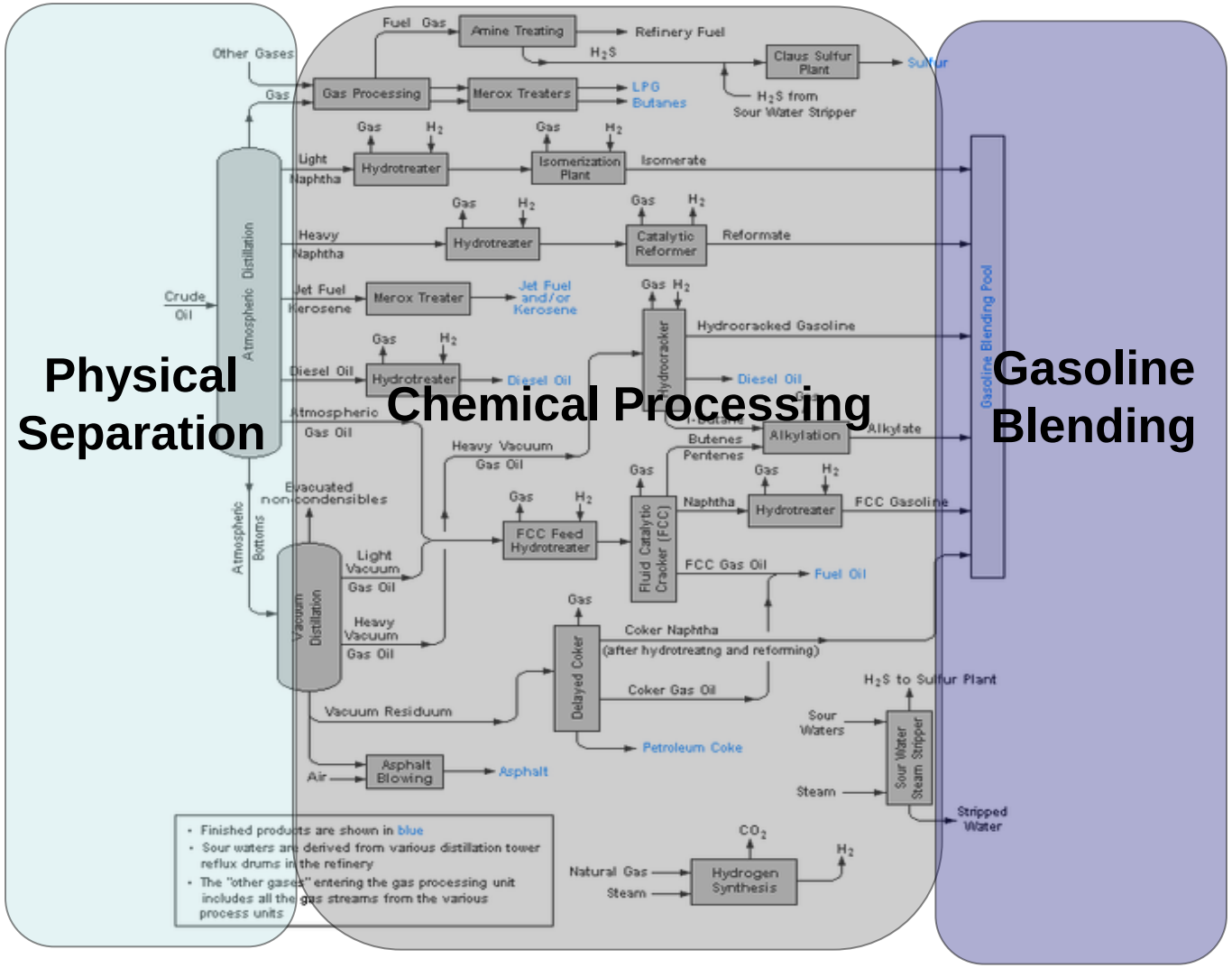
Typical Oil Refinery



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Blending to Specifications

Table of key specifications for commercial gasoline, as set out by EN-228

Property	Units	Minimum	Maximum	
Density at 15°C	kg/m^3	720	775	
Research Octane Number		95		Chemical
Motor Octane Number		85		
Summer Vapour Pressure	kPa	45	60	Physical
Distilation (1013 mbar)	%vol	20	48	
Distillation Residue	%vol		2	
Final Boiling Point	°C		210	
Copper Strip Corrosion (3h at 50°C)	Rating	Class 1		
Oxidation Stability	hrs	6		
Olefins	% vol		18	
Aromatics	% vol		35	
Benzene	% vol		1	
Oxygen	% wt		2.7	
Ethanol	% vol		5	
Tert-butyl alcohol	% vol		7	
Sulphur	% vol		10	

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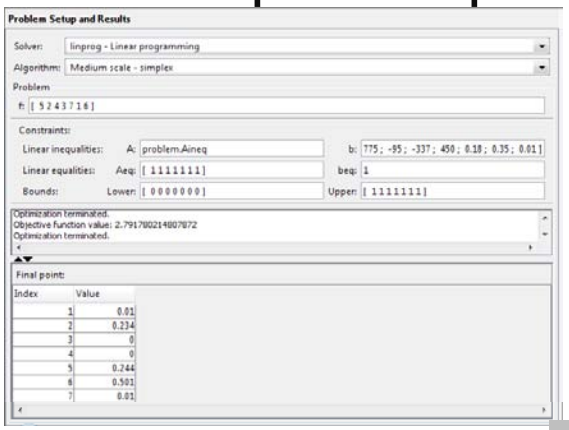
Overview

Optimisation Programme

- Use cost to indicate carbon intensity of fuel
- Octane number important parameter.



Knowledge of Blending Pots

Octane Tests

Chemical Kinetic Fuel Model

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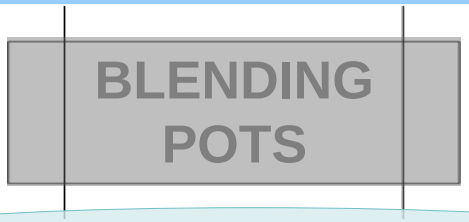
Choice of Chemical Surrogates

- **PARAFFINS**
  - C4-C7 range
- **NAPHTHENES**
  - C6 – C7 range
- **OLEFINS**
  - C5 – C7 range
- **AROMATICS**
  - C6 – C8 range
- **OXYGENATES**
  - Ethanol or MTBE
- **ANTI-KNOCK**



ETBE	Ethanol
C3 Alkylate	N-heptane
C4 Alkylate	Iso-octane
Cat Cracked Light Naphtha	N-butane
Cat Cracked Heavy Naphtha	Toluene
Isomerate	Methyl-cyclohexane
Reformate	Di-isobutylene

SURROGATE SPECIES

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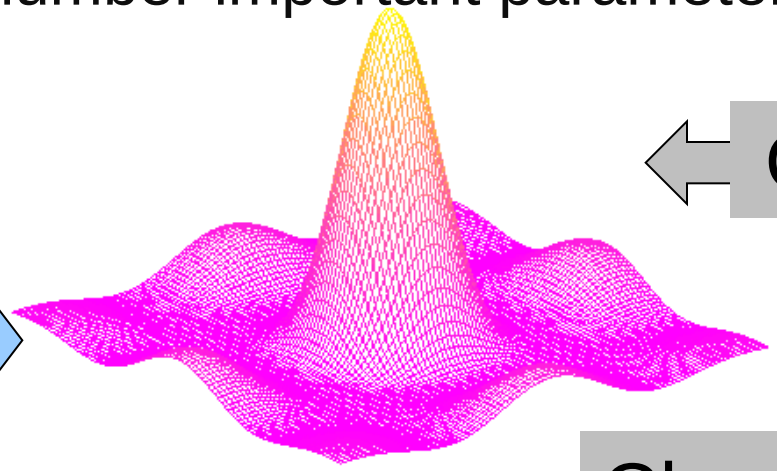

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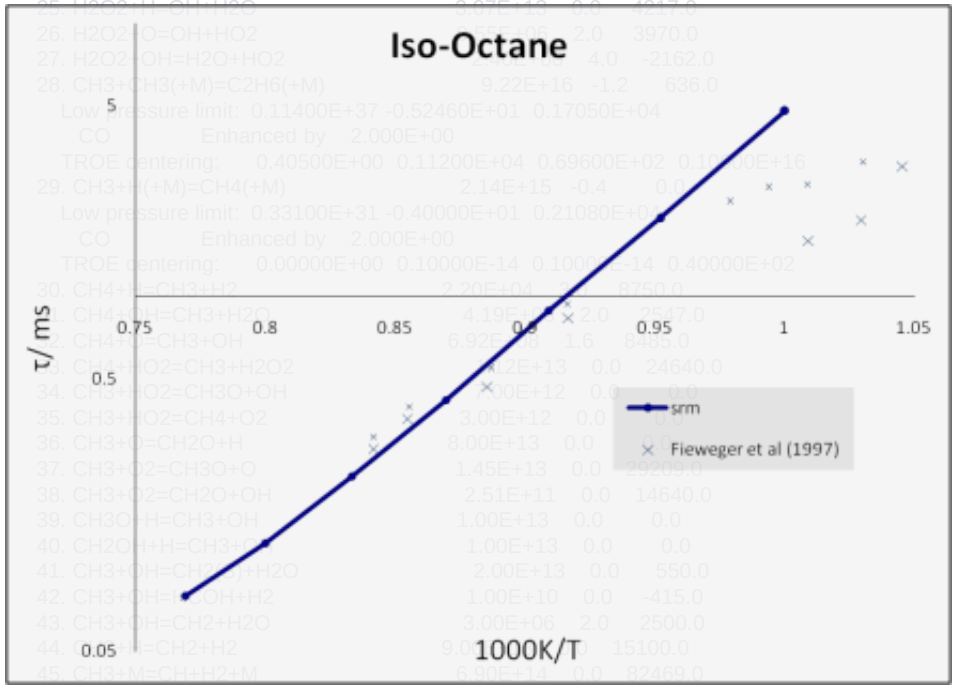
Chemical Kinetic Fuel Model

- Reduced mechanism for iso-octane, n-heptane, toluene and ethanol chosen as base mechanism.
- Di-isobutylene, methylcyclohexane and butane added.



- Resulting model contains **215 chemical species** and **1192 chemical reactions.**

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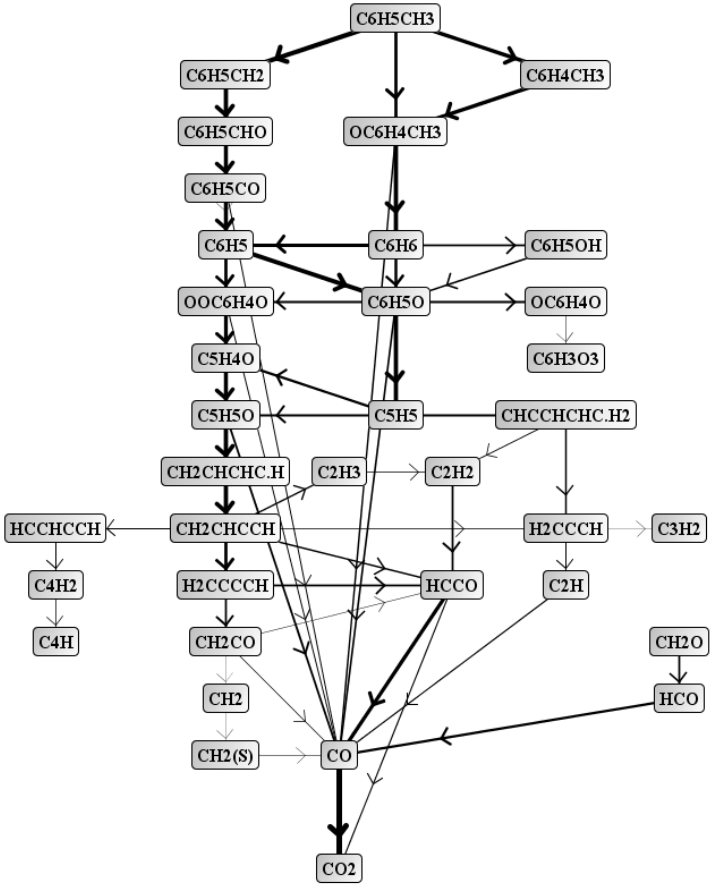
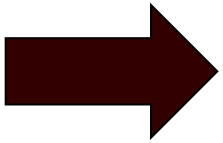
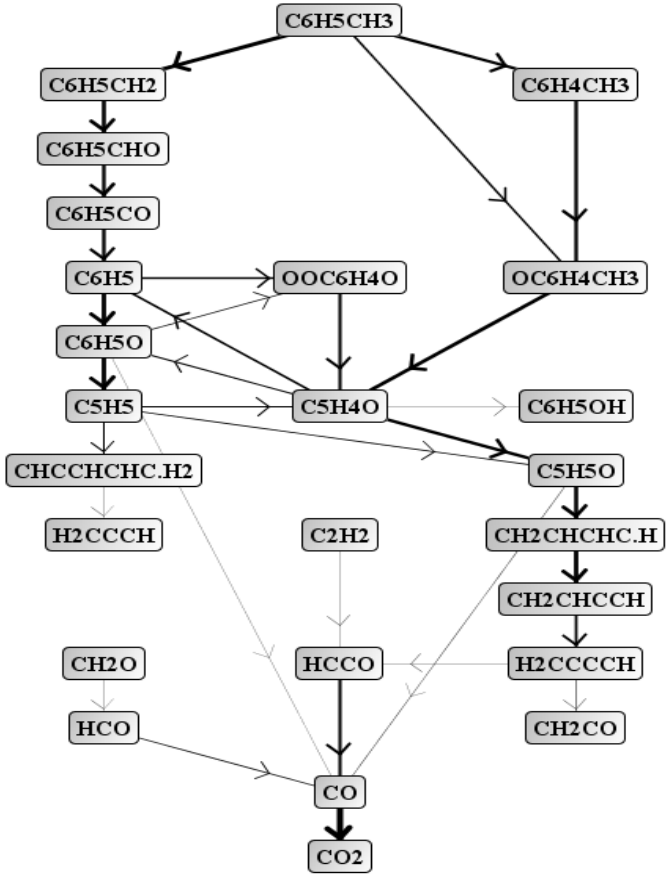
Mechanism Reduction



Toluene Flux: Full Mechanism

Removal of species and reactions





Toluene Flux: Skeletal Mechanism

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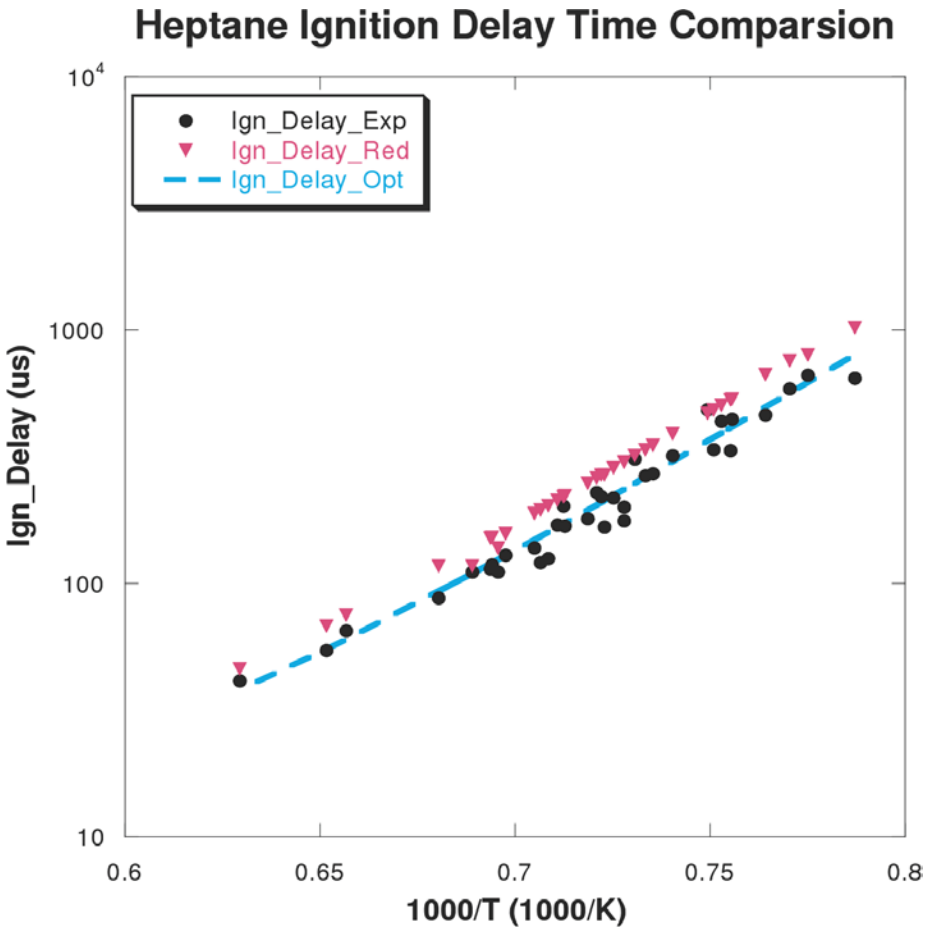
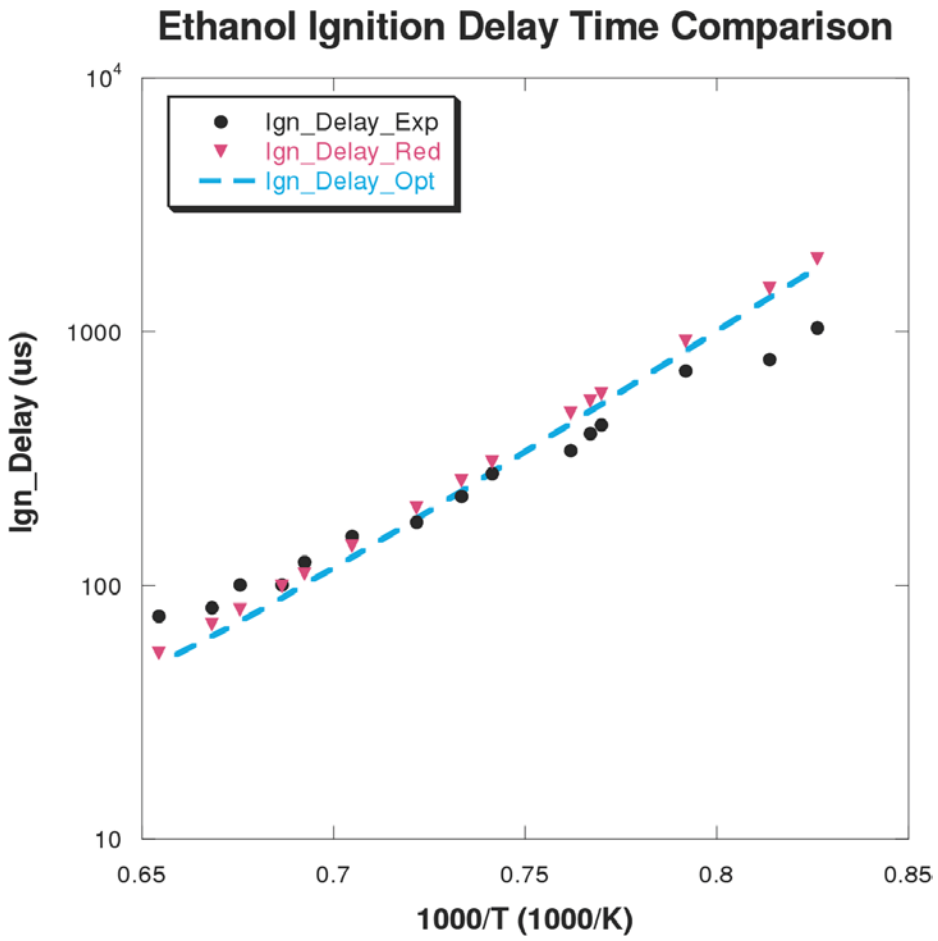
Fuel Model Optimisation





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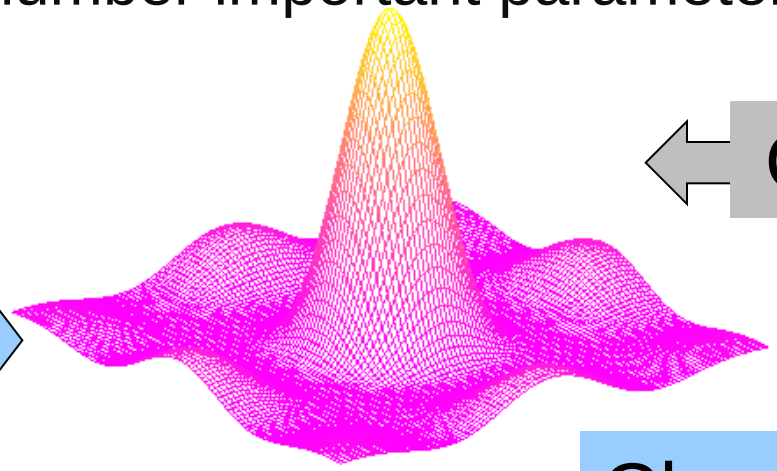
Overview

Optimisation Programme

- Use cost to indicate carbon intensity of fuel
- Octane number important parameter.



Octane Tests

Knowledge of Blending Pots

Chemical Kinetic Fuel Model

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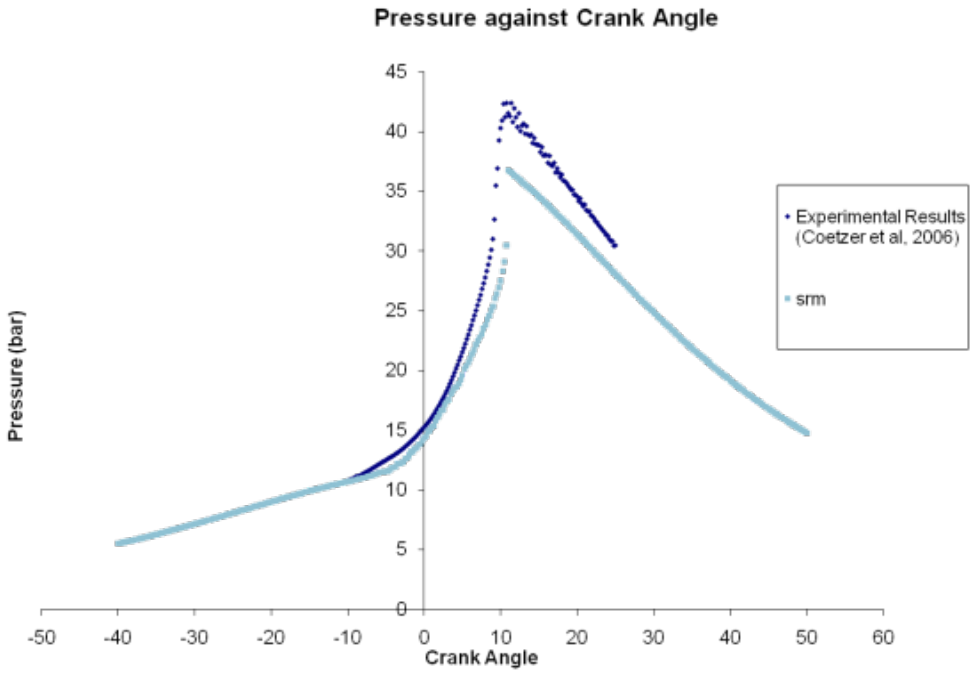
Modelling Octane Number

- Industrially, octane number determined using engine test.
- Model used to predict octane number from fuel composition.



- Engine test required to predict octane number accurately.

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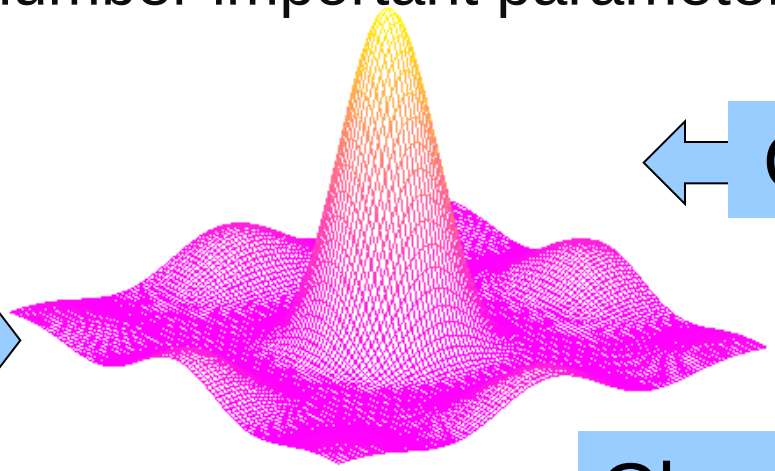
Further Work

Optimisation Programme

- Use cost to indicate carbon intensity of fuel
- Octane number important parameter.



Octane Tests

Knowledge of Blending Pots

Chemical Kinetic Fuel Model

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Thank you