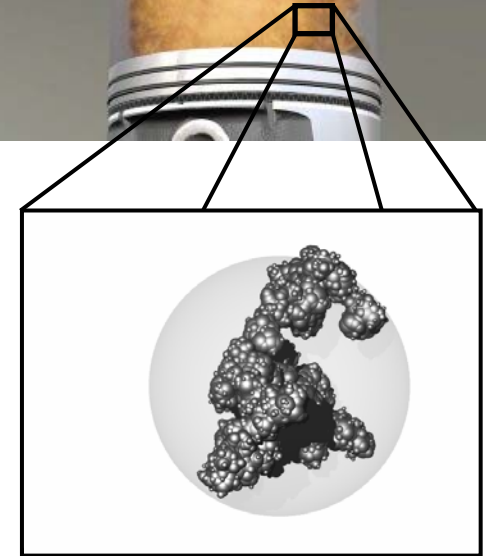
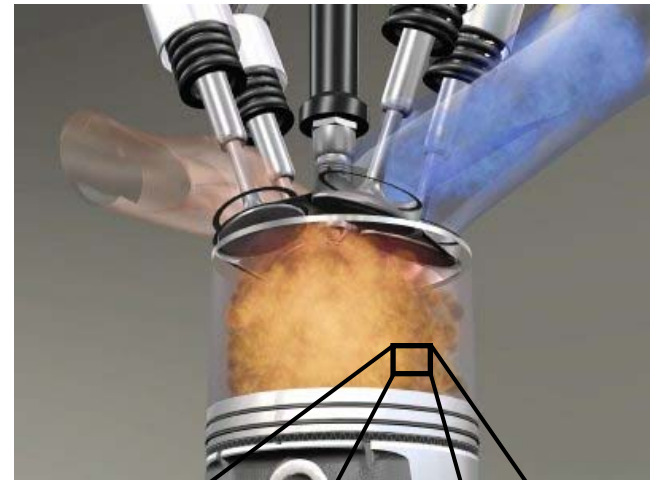


Soot modelling in direct injection spark ignition and diesel engines

Jonathan Etheridge, Sebastian Mosbach,
Andreas Braumann, George Brownbridge,
Andrew Smallbone, Amit Bhave, Markus Kraft,
Hao Wu, Nick Collings
University of Cambridge

Antonis Dris, Robert McDavid
Applied Research Europe, Caterpillar Inc.



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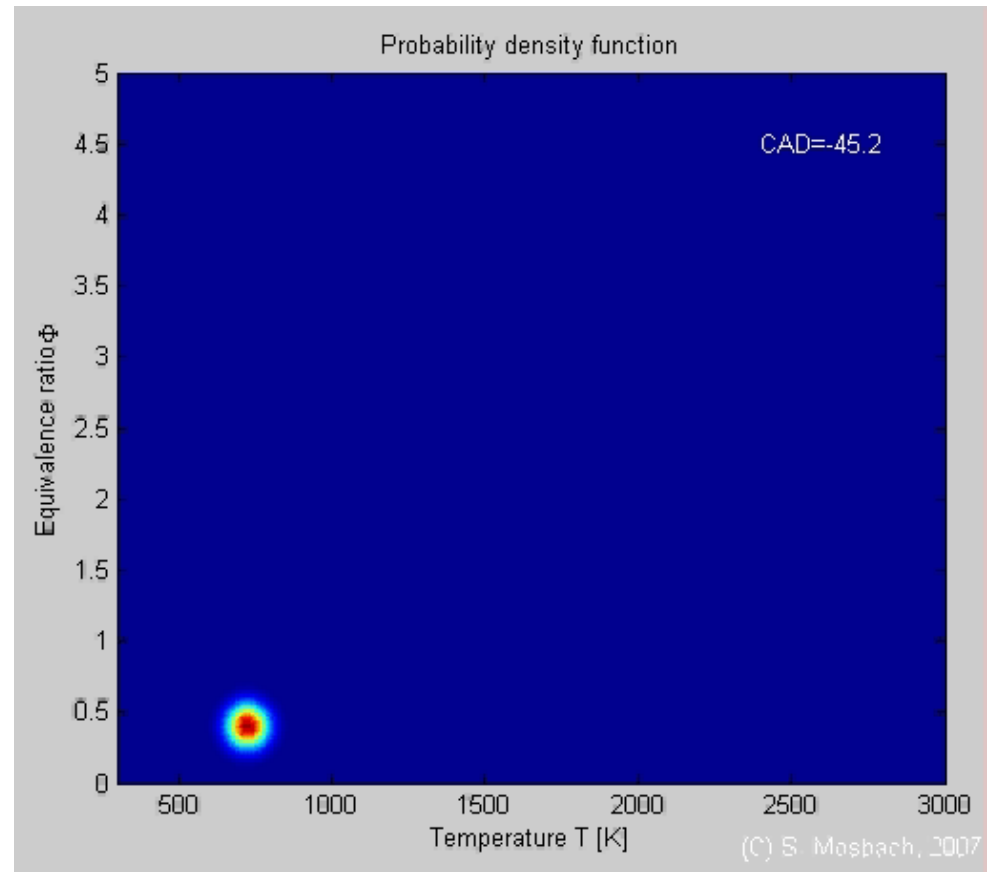
21st May 2010



CATERPILLAR
**UNIVERSITY OF
CAMBRIDGE**

Stochastic Reactor Model (SRM)

- Simulates closed-volume in-cylinder processes.
- Models turbulent mixing, convective heat transfer, direct injection, spark ignition, soot formation.
- Detailed chemical mechanism for PRF + NOx + soot precursors (208 species, 1002 reactions).



Test case:

PFI and DI at 40 CAD BTDC

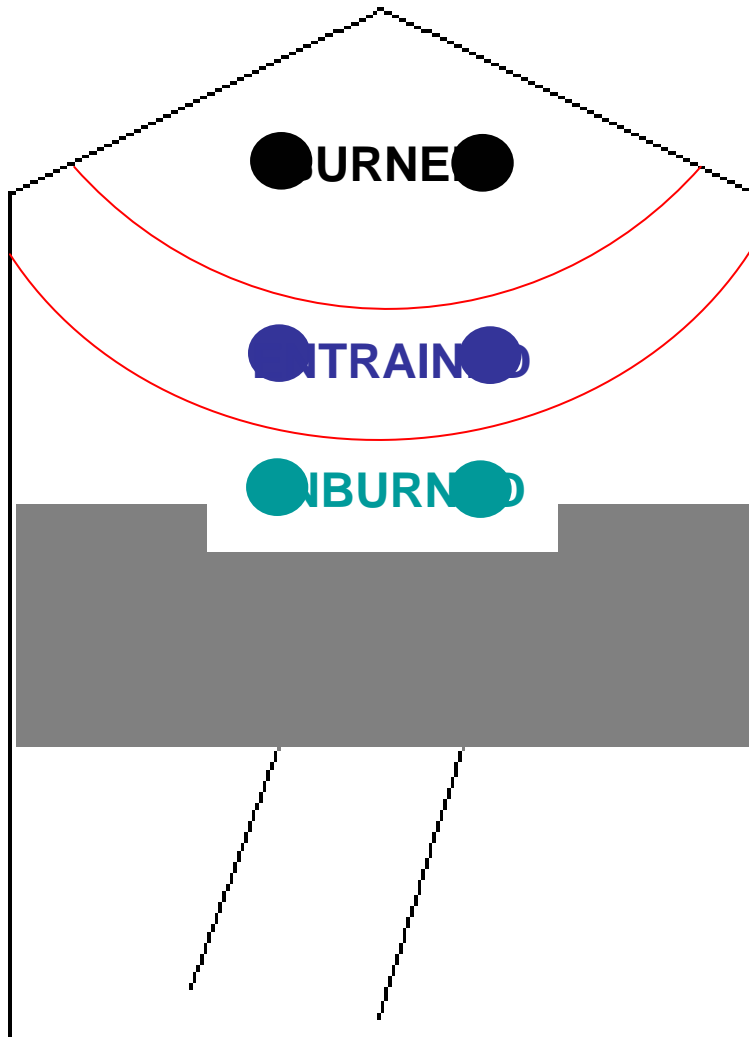


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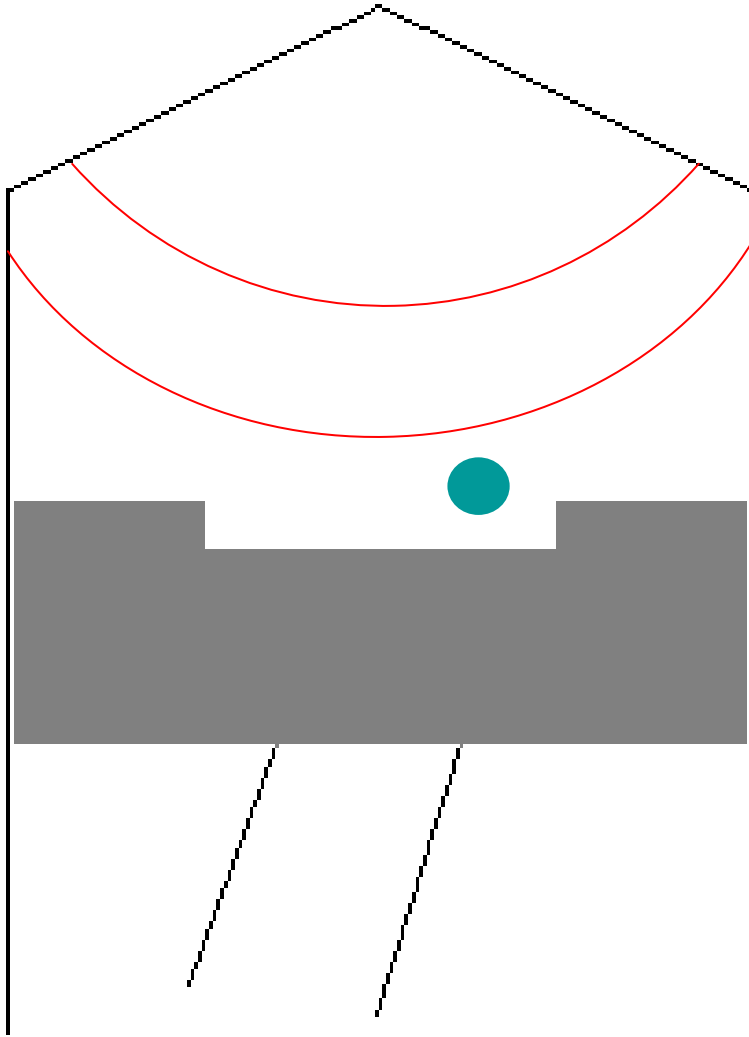
SI model



- The model contains three zones.
- Mixing occurs within each zone but not between zones.



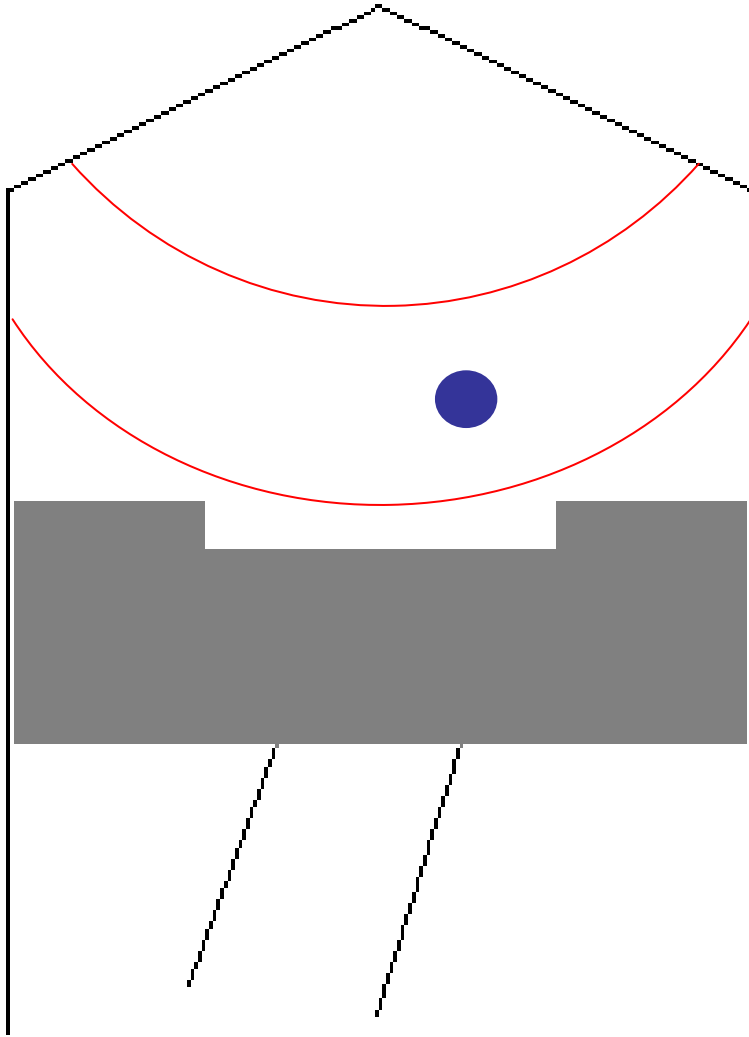
SI model



- The turbulent flame speed is used to calculate the new flame radius.
- When the calculated volume is greater than the particles' volume a new particle is added to the entrained zone.



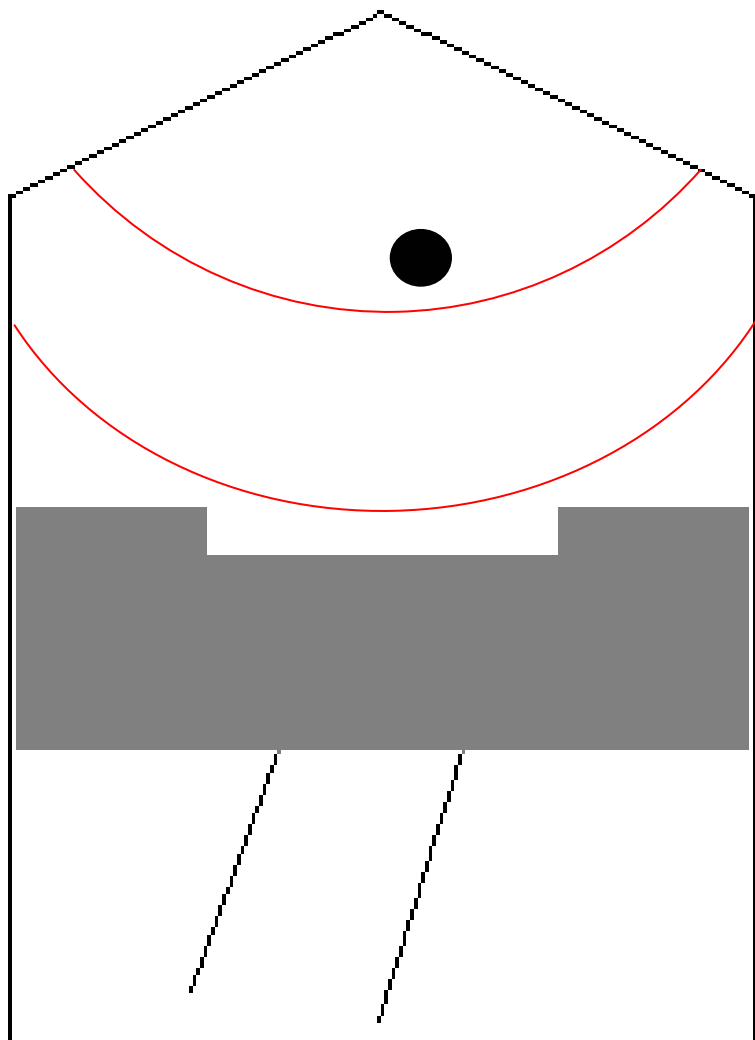
SI model



- Particles move from entrained to burned zone once heat release rate goes above then drops below a certain value.



SI model

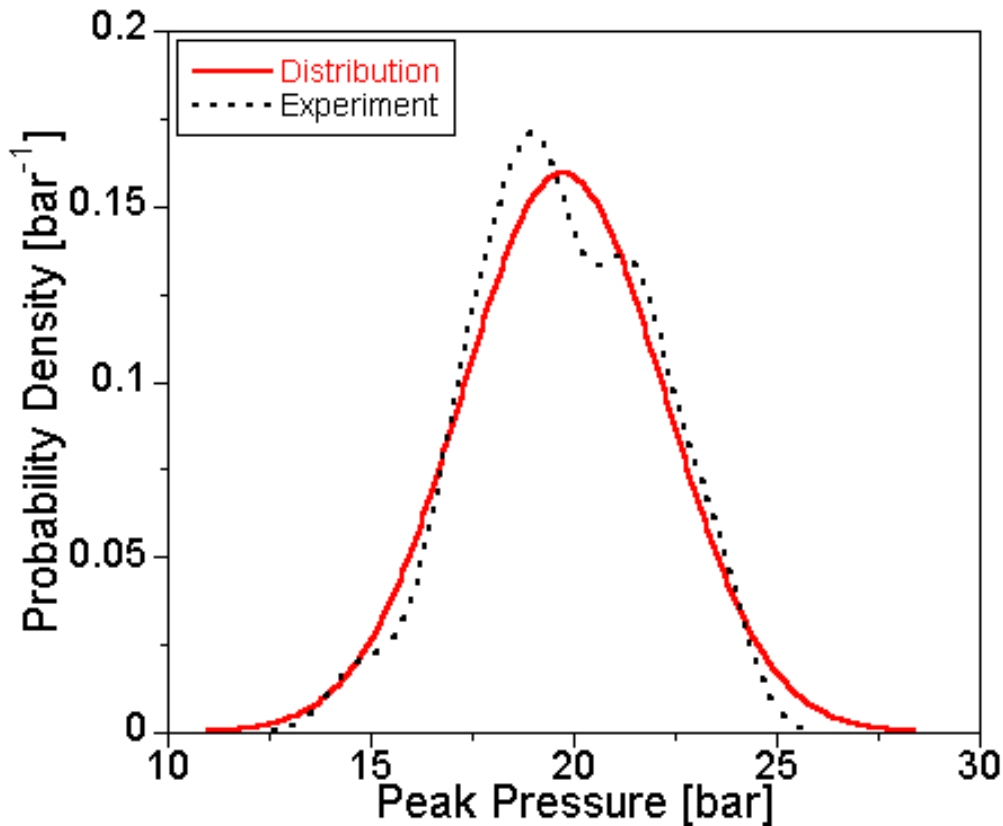


- The chemistry within each particle is calculated at each time step with the detailed mechanism.



SI engine CCV

Cycle-to-cycle variation (CCV)



Fuel	gasoline
Bore	87.5 mm
Stroke	83.0 mm
Con. rod length	146.3 mm
Disp. volume	499 cm ³
CR	12.0
Speed	1500 RPM
Air/fuel equiv. ratio	1.0
EGR	28.8%



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ENGINEERING

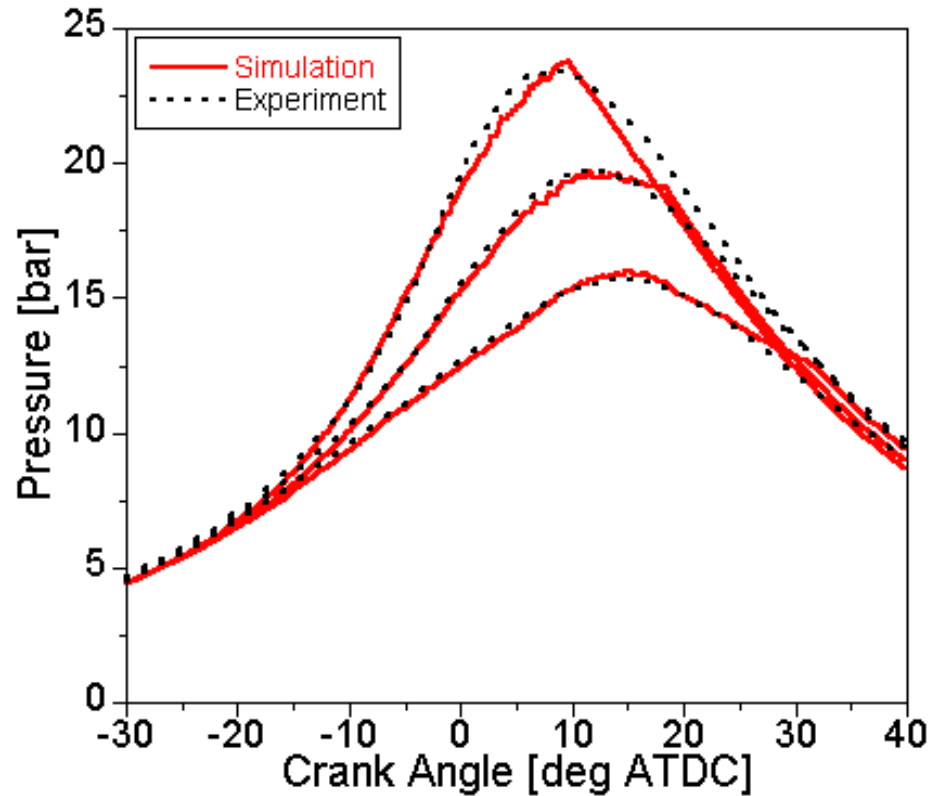


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SI model calibration



- Characteristic flame speed obtained from:

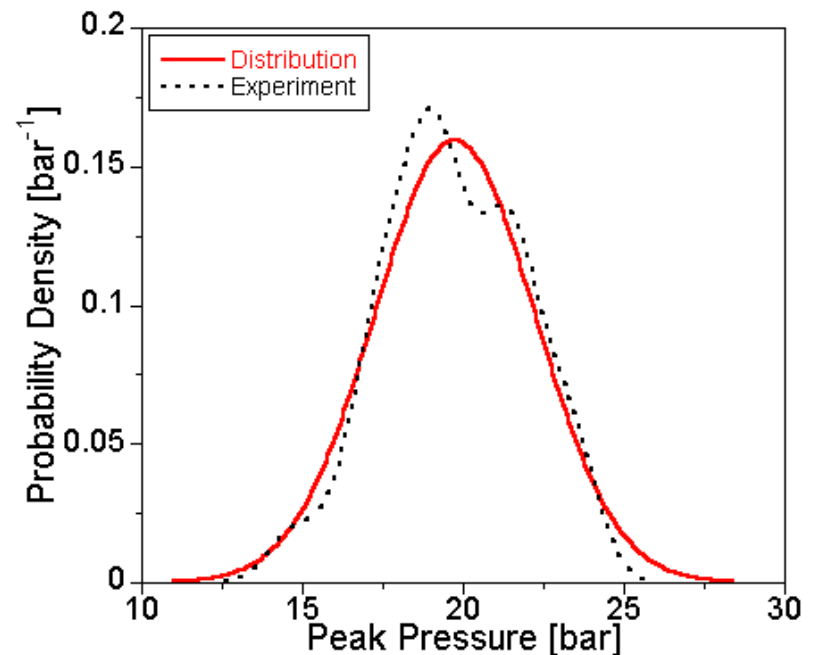
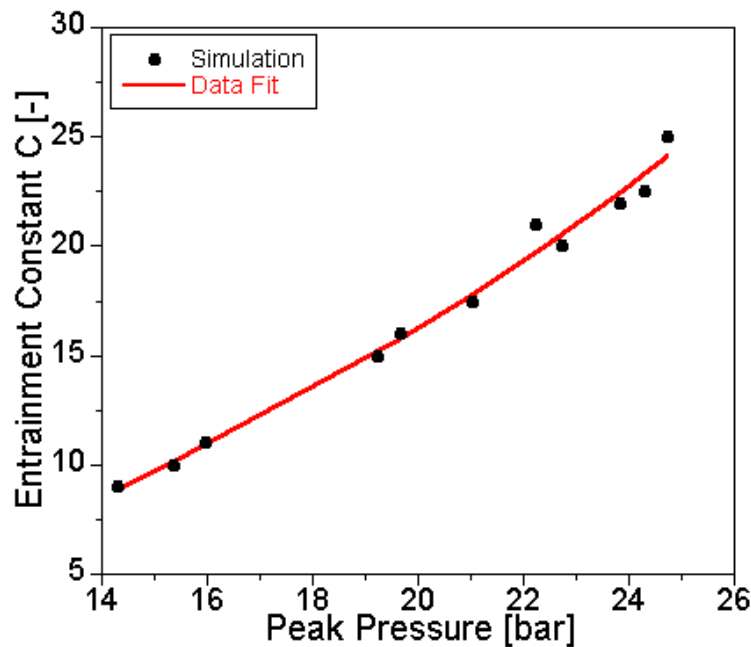
$$u_T = 0.08C\bar{u}_i \left(\frac{\rho_u}{\rho_i} \right)^{1/2}$$

- Constant, C, calibrated to match representative slow, medium and fast cycles.

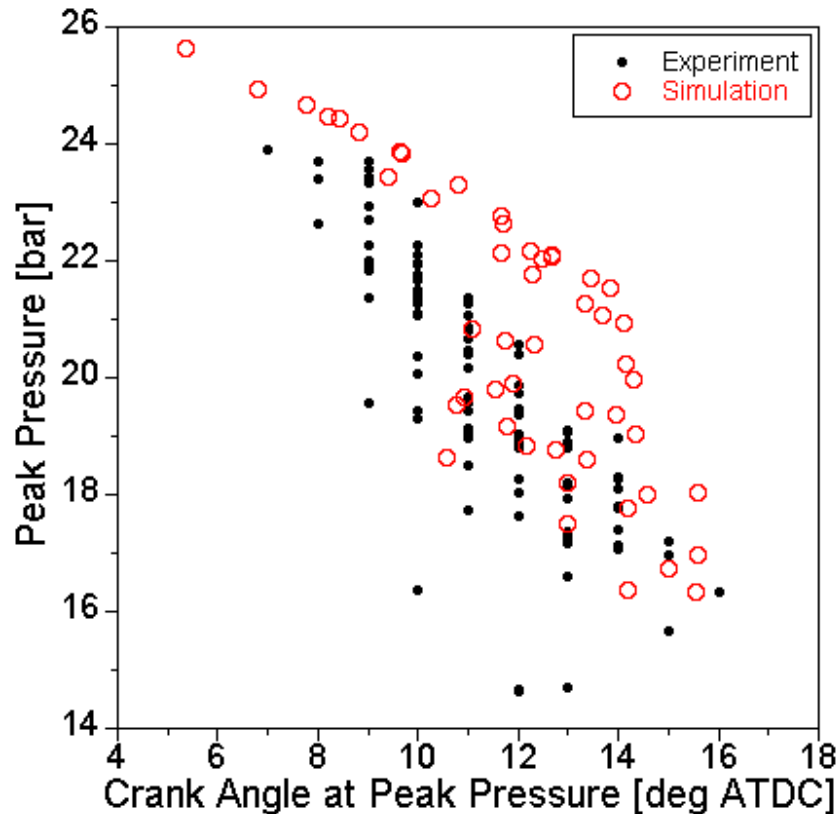


SI model calibration

- Relation between C and the peak pressure obtained.
- Used with peak pressure distribution to provide C during each cycle of a multi-cycle simulation.



Multi-cycle SI simulation



- Model coupled to GT-Power for multi-cycle simulation.
- 50 simulated and 96 experimental cycles.
- NO_x emissions:
 - 790 ppm simulation
 - 530 ppm experiment



DISI engine



- Late injection produces stratified mixture.
- Fuel rich regions close to spark gap.

Image from www.engineforall.com



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DISI engine experiments

- Data from Maricq *et al.*, SAE 1999-01-1530.
- Fuel comprised of 60% paraffin and 40% aromatic compounds.
- Fuel modelled as 60% iso-octane and 40% toluene.
- Exhaust measurements for various injection timings.

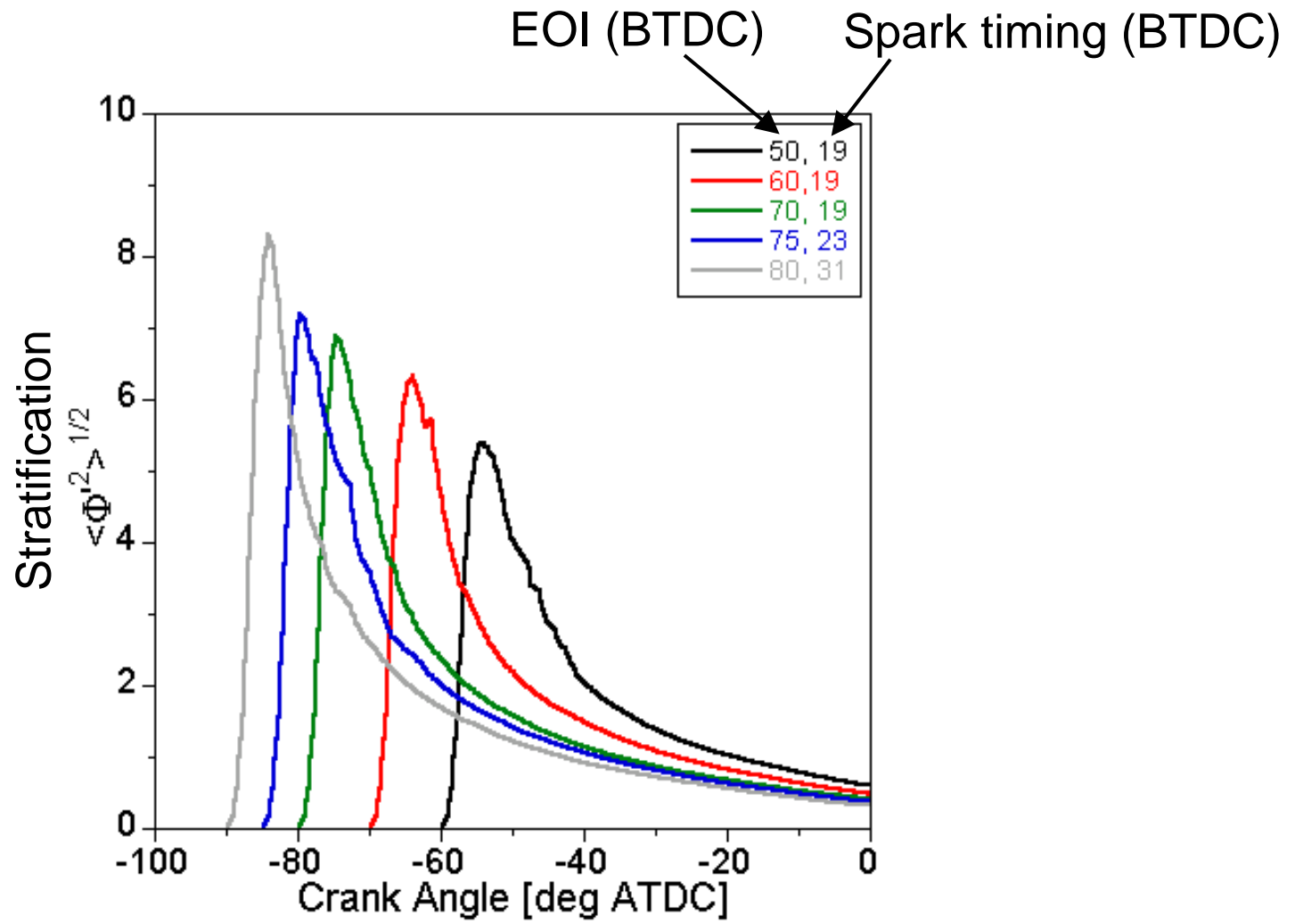
Cylinders	4
Bore [mm]	81.0
Stroke [mm]	89.0
Disp. volume [cm ³ /cyl]	457.5
Compression Ratio	12

1500 RPM, $\Phi=0.58$ (global)

Case	1	2	3	4	5
EOI [CAD ATDC]	-50	-60	-70	-75	-80
Spark Timing [CAD ATDC]	-19	-19	-19	-23	-31

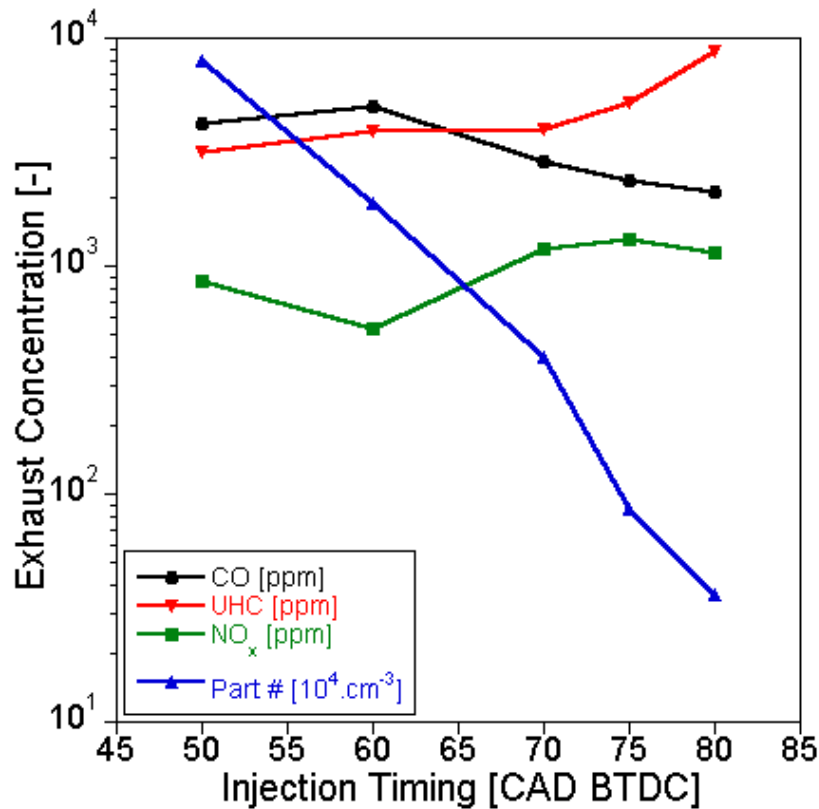


DISI engine simulation results

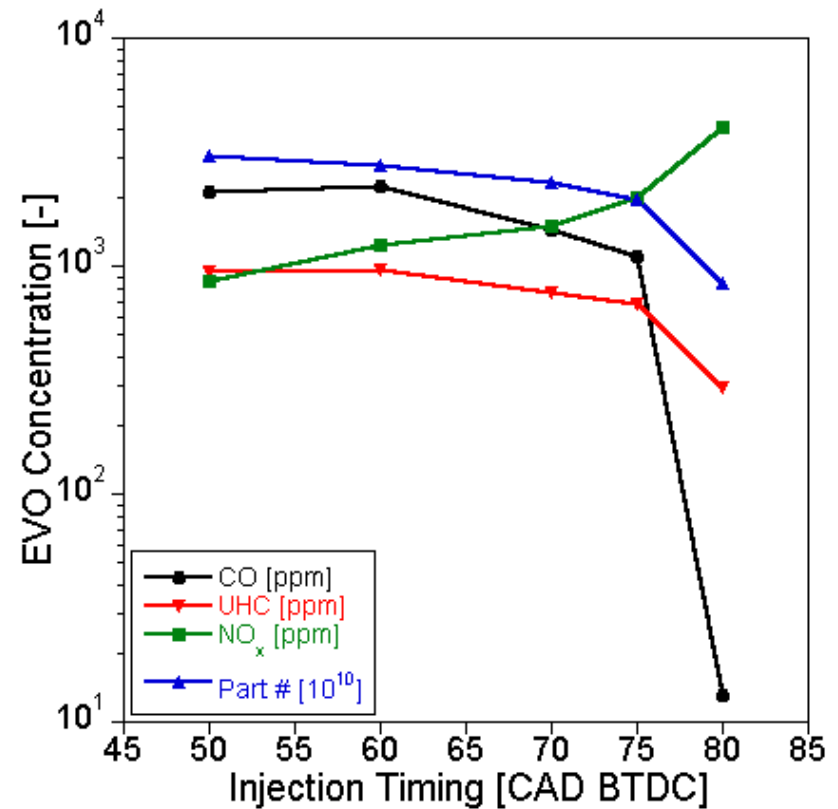


DISI engine emissions

Experiment

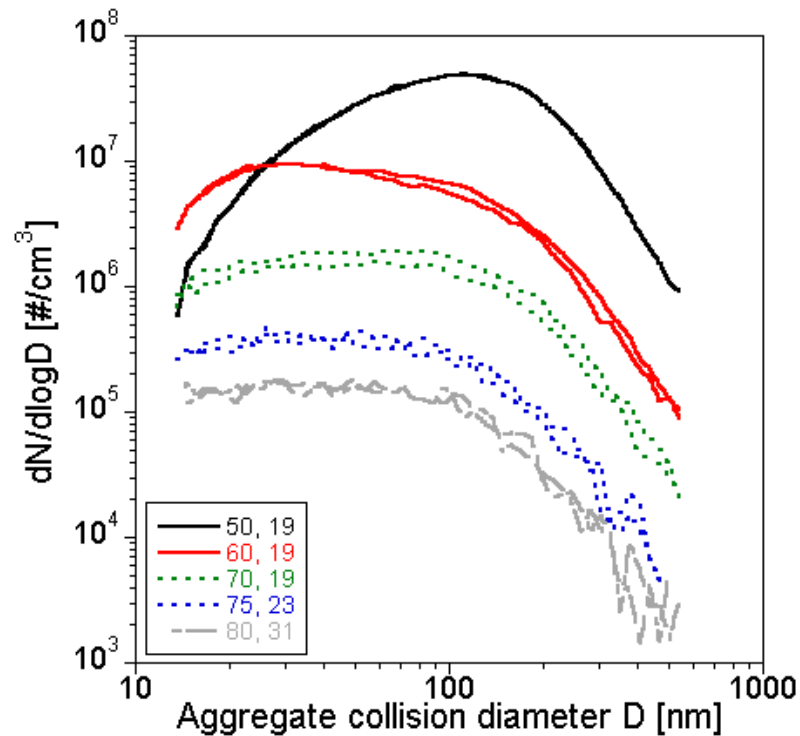


Simulation

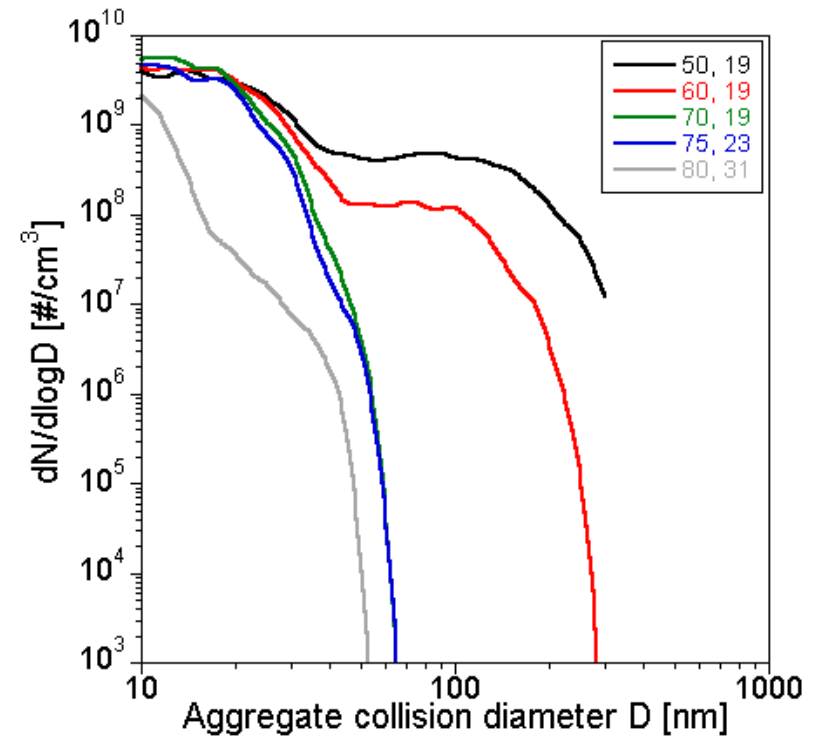


Particle size distributions

Experiment



Simulation

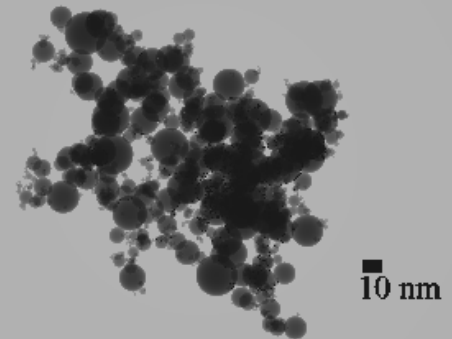
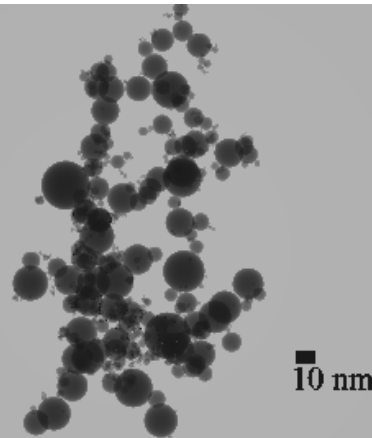
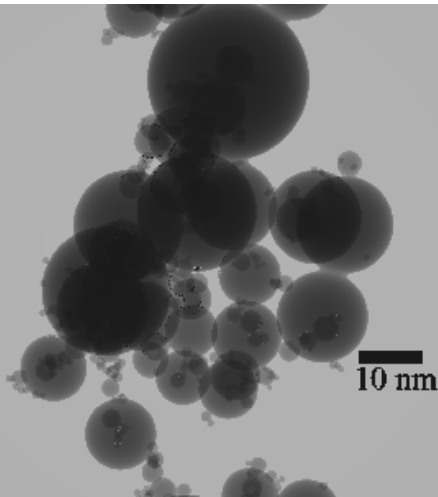


Soot in DISI engine

2.6 CAD ATDC

12.6 CAD ATDC

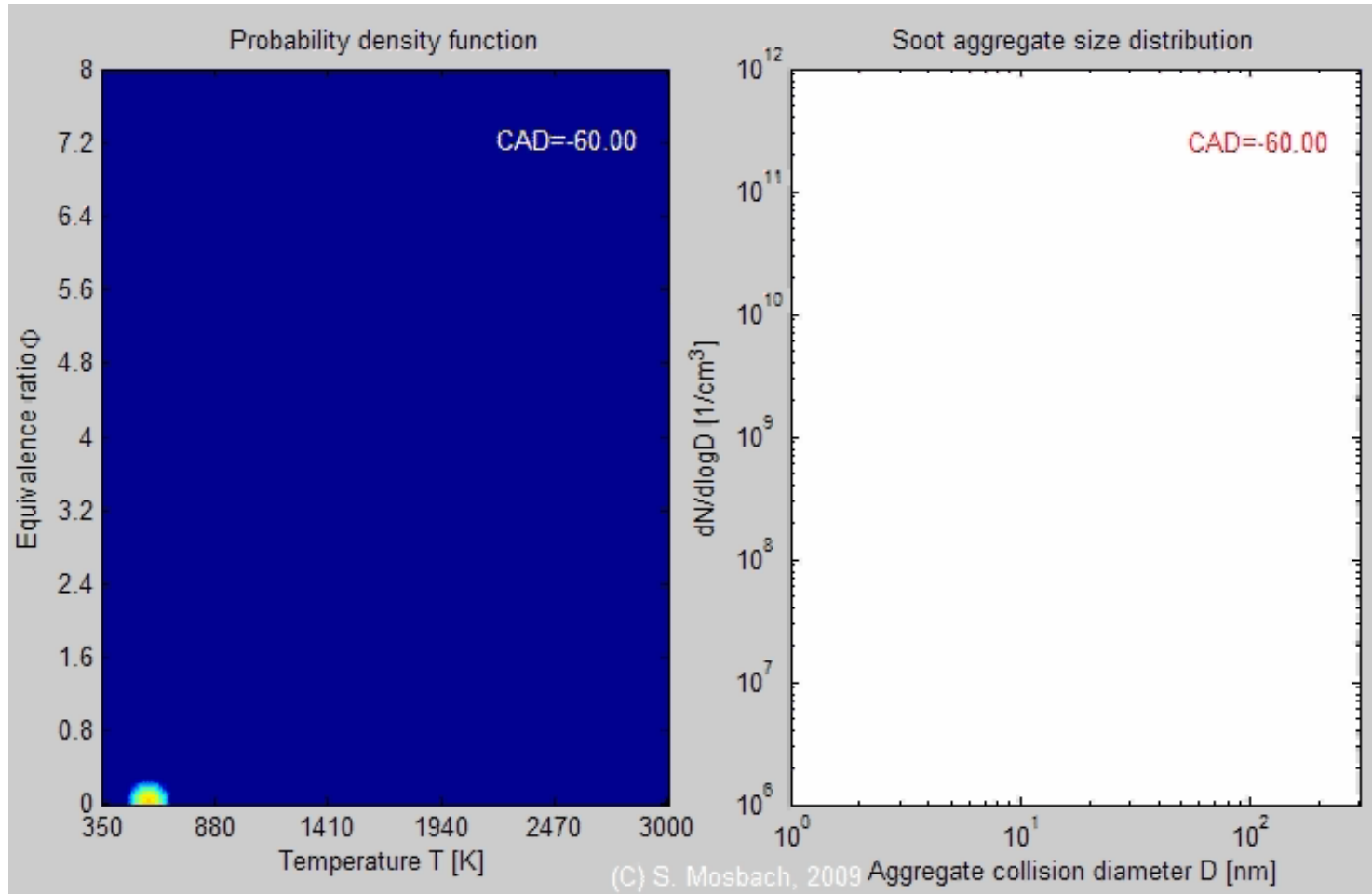
32.6 CAD ATDC



CAD [deg ATDC]	2.6	12.6	32.6
No. Primaries	492	1315	2083
Coll. Diam [nm]	70	108	137



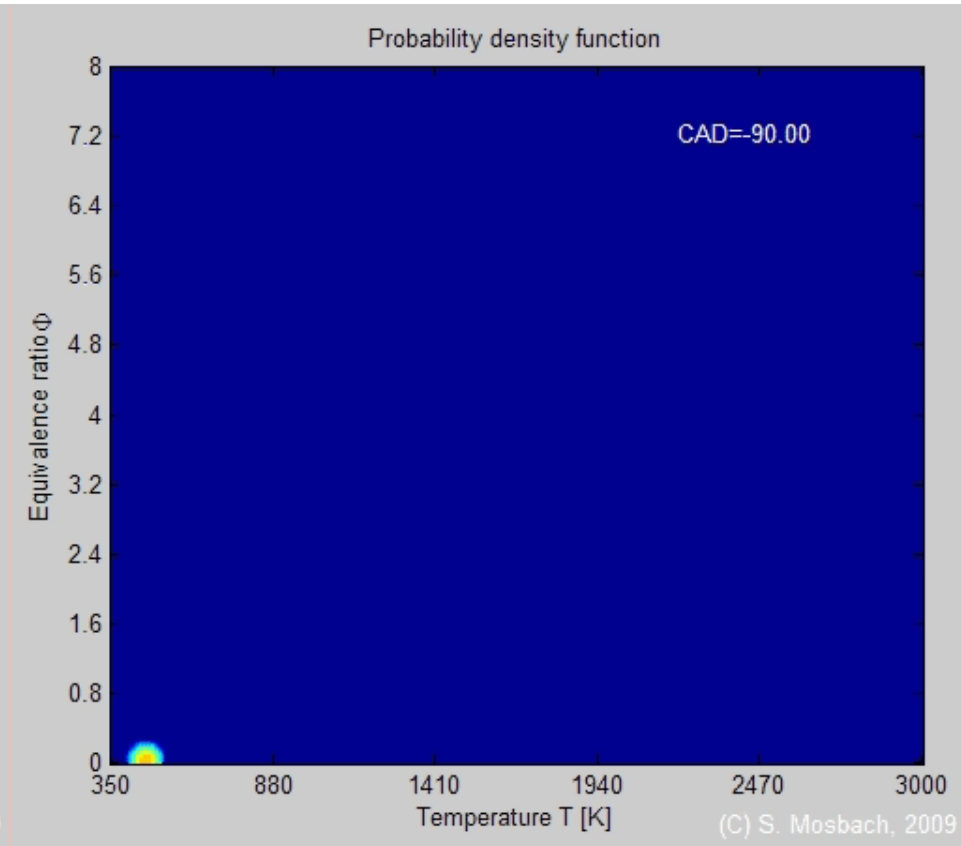
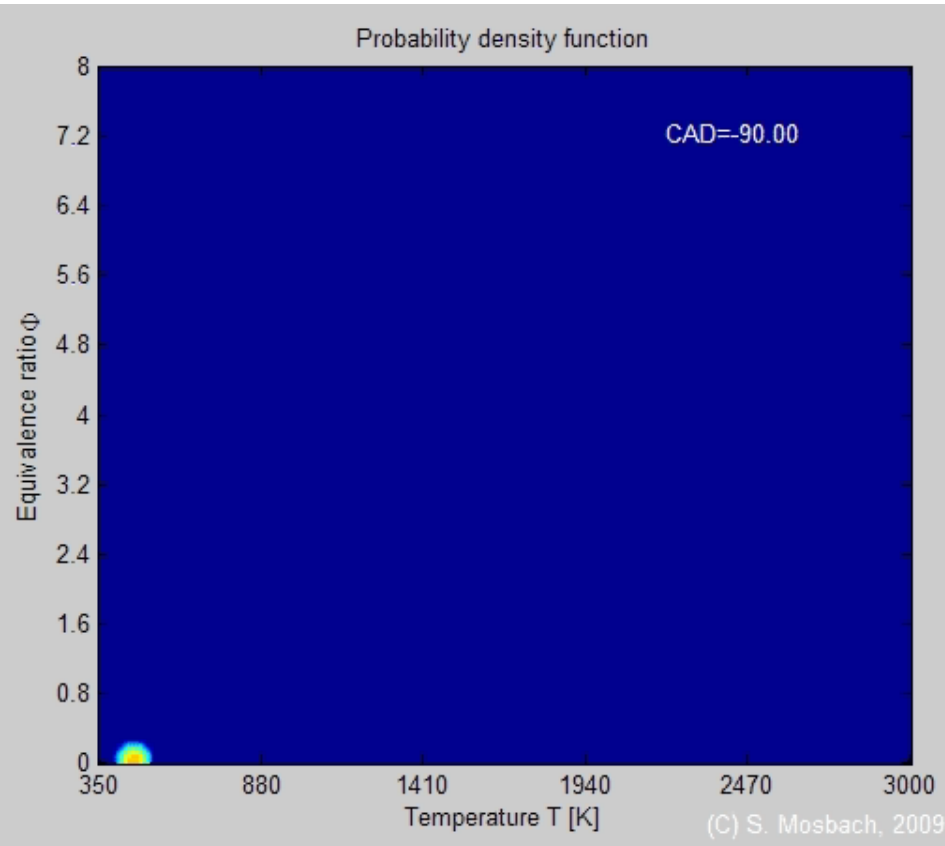
Temporal evolution (late injection)



Comparison early/late injection

EOI -80 CAD ATDC
Spark -31 CAD ATDC

EOI -50 CAD ATDC
Spark -19 CAD ATDC



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Problem

Current engine model development

- Experimental data in a variety of formats, sometimes largely unstructured, often incomplete
- Uncertainties/errors associated with experimental data typically unknown or unavailable
- Too many models and “tuneable”/unknown model parameters
- How “good” (or not) is a particular model?

=> Ad hoc, fragmented, short-term approach



Solution: Process Informatics

We need a robust **integrated methodology** to help us work systematically and efficiently:

- Effective use of cost-intensive experimental data through **data standardisation**
- Systematic and robust model development through **systematic optimisation**, taking into account **uncertainties**
- Suggesting “useful” future experiments



A data model: engineML

Consistent format

- point data (e.g. rpm, CO, u_i)
- time resolved data (p -CA)
- apparatus (production engine, research engine)
- errors
- data type (consistent units)
- raw or processed
- experimental or model

eXtensible Markup Language (XML)

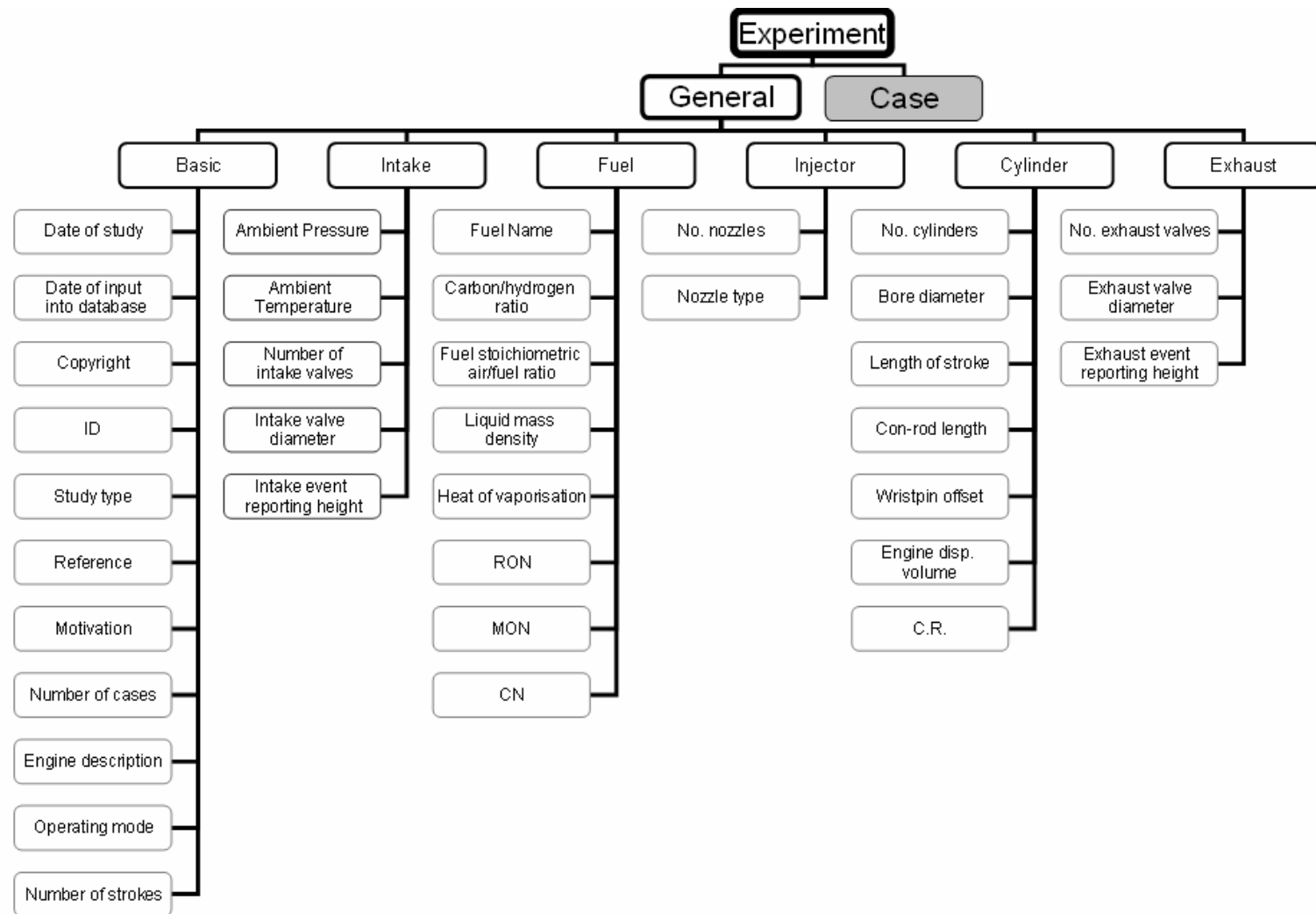
- machine and human readable, tagged with metadata
- highly structured (tree), easily queried
- can be validated against schema

Easily accessible database

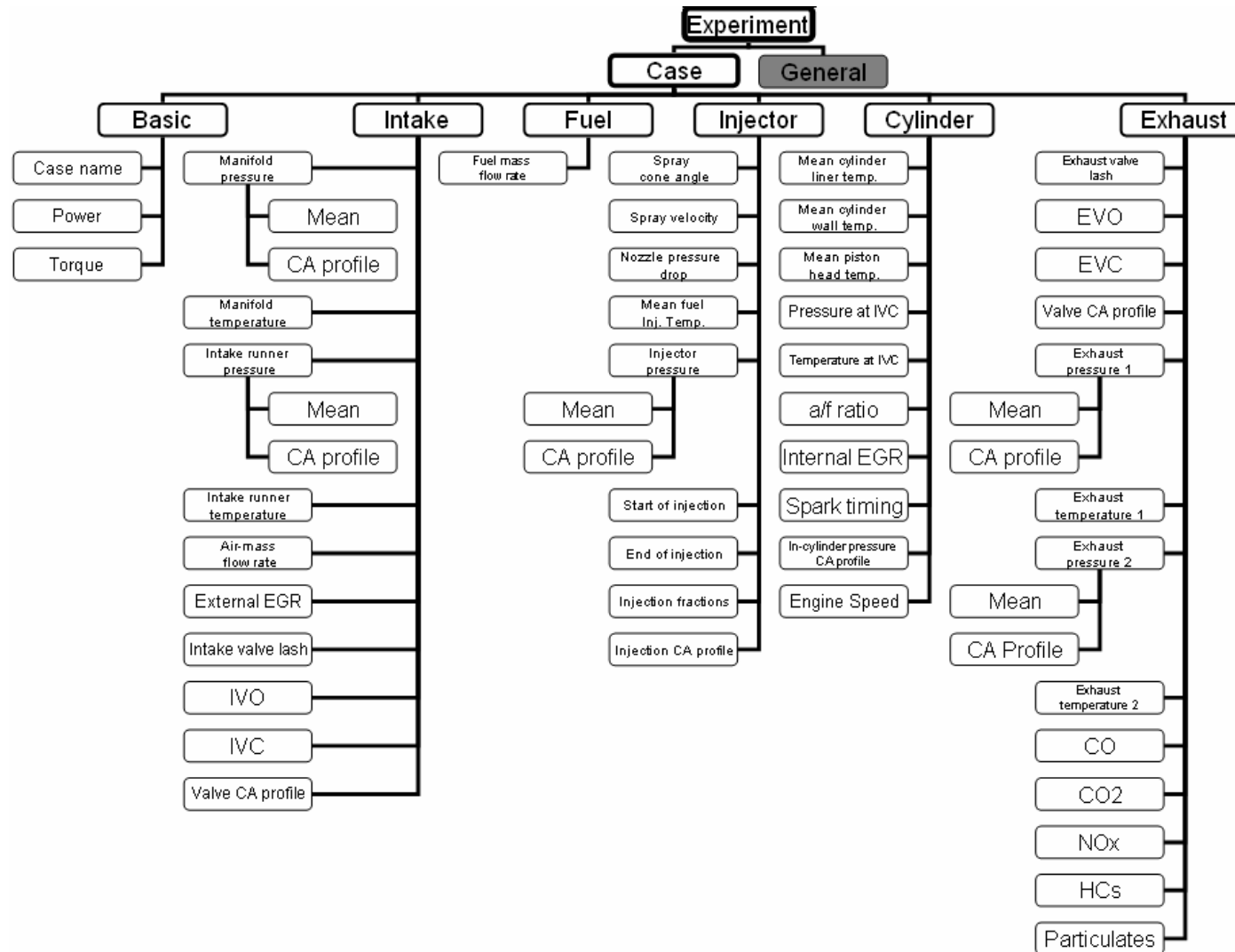
- read by model code
- data stored consistently
- old data never “lost”



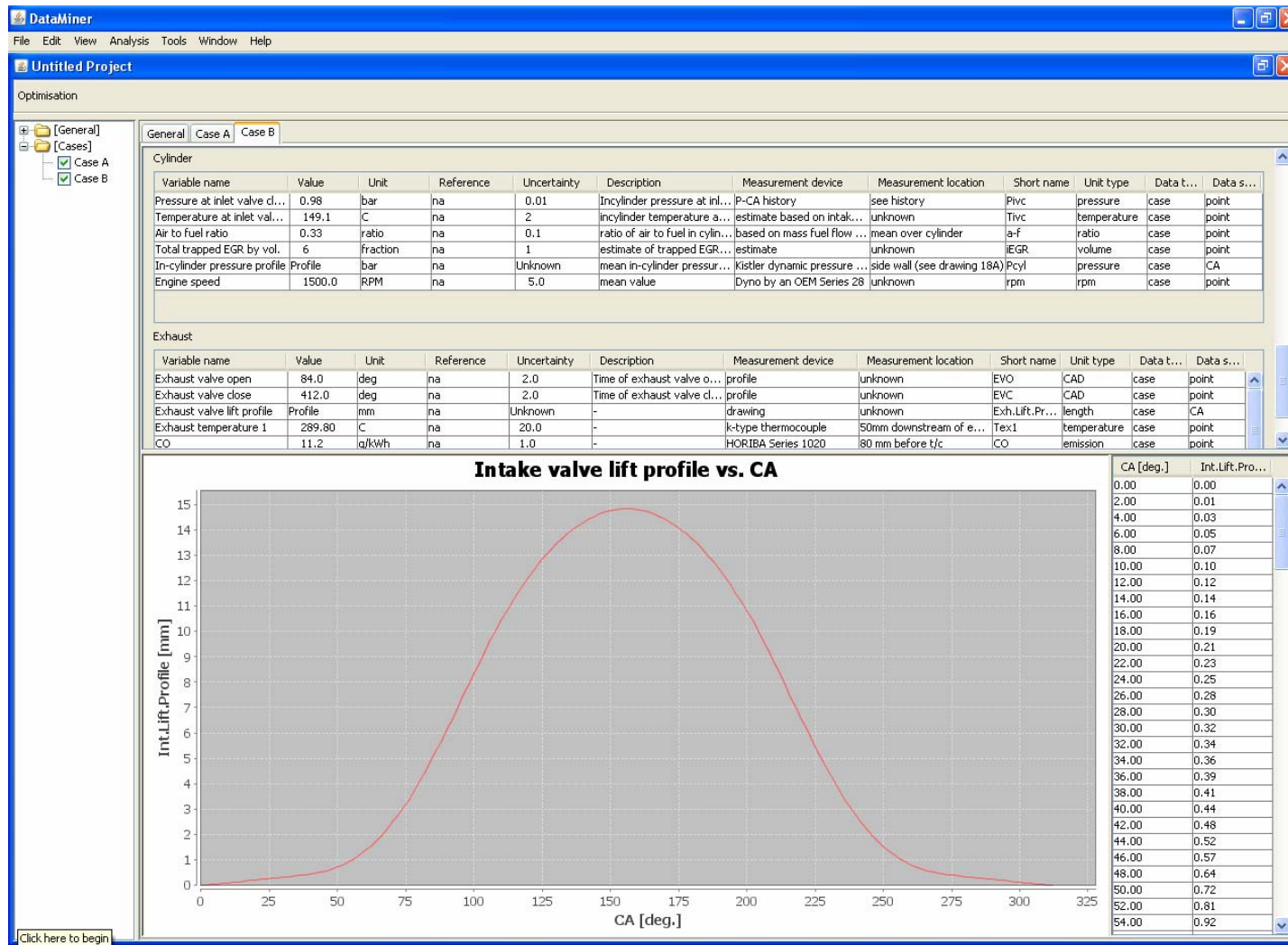
General data



Case data



Data visualisation



Model parameter optimisation

We must accept that model parameters exist and have to be tuned to experimental data!

What is the best way to fit these parameters?

- As many data points as possible
- Uncertainties in experimental data as well as model parameters must be accounted for
- Use experimental data to reduce model parameter uncertainties
- Use experimental and model uncertainties to identify possible outliers in the data, or model shortcomings

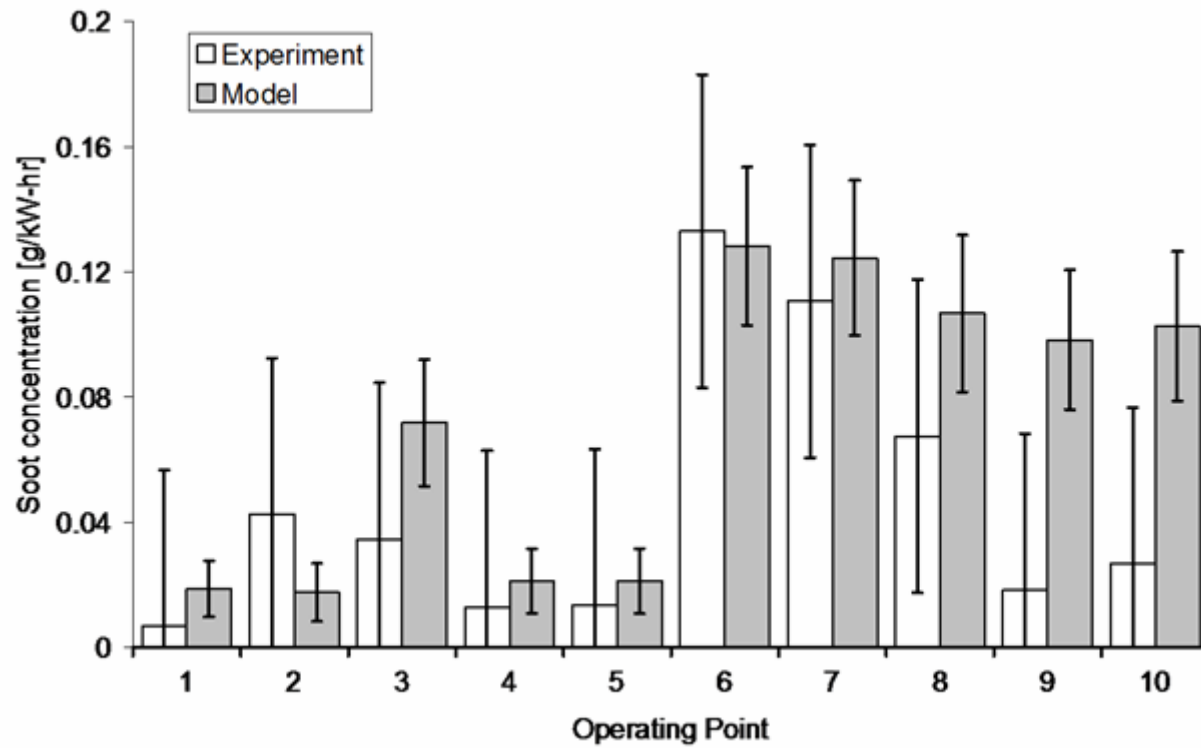


Application: Diesel soot

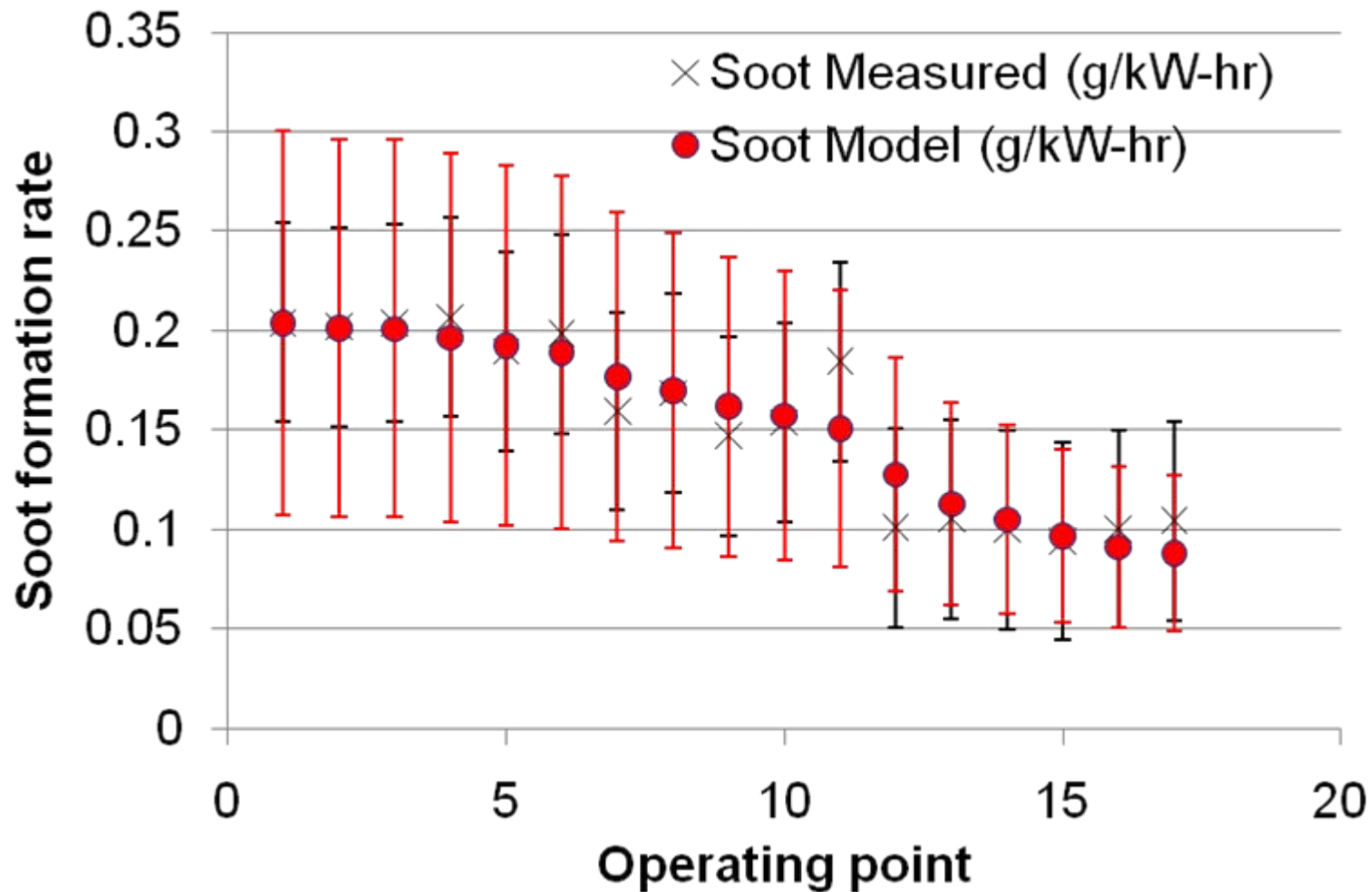
Empirical soot model (Plee):

$$\text{soot}[g] = A \cdot \text{mps}^B \cdot \text{phi}^C \cdot \exp\left(\frac{D}{T_f}\right)$$

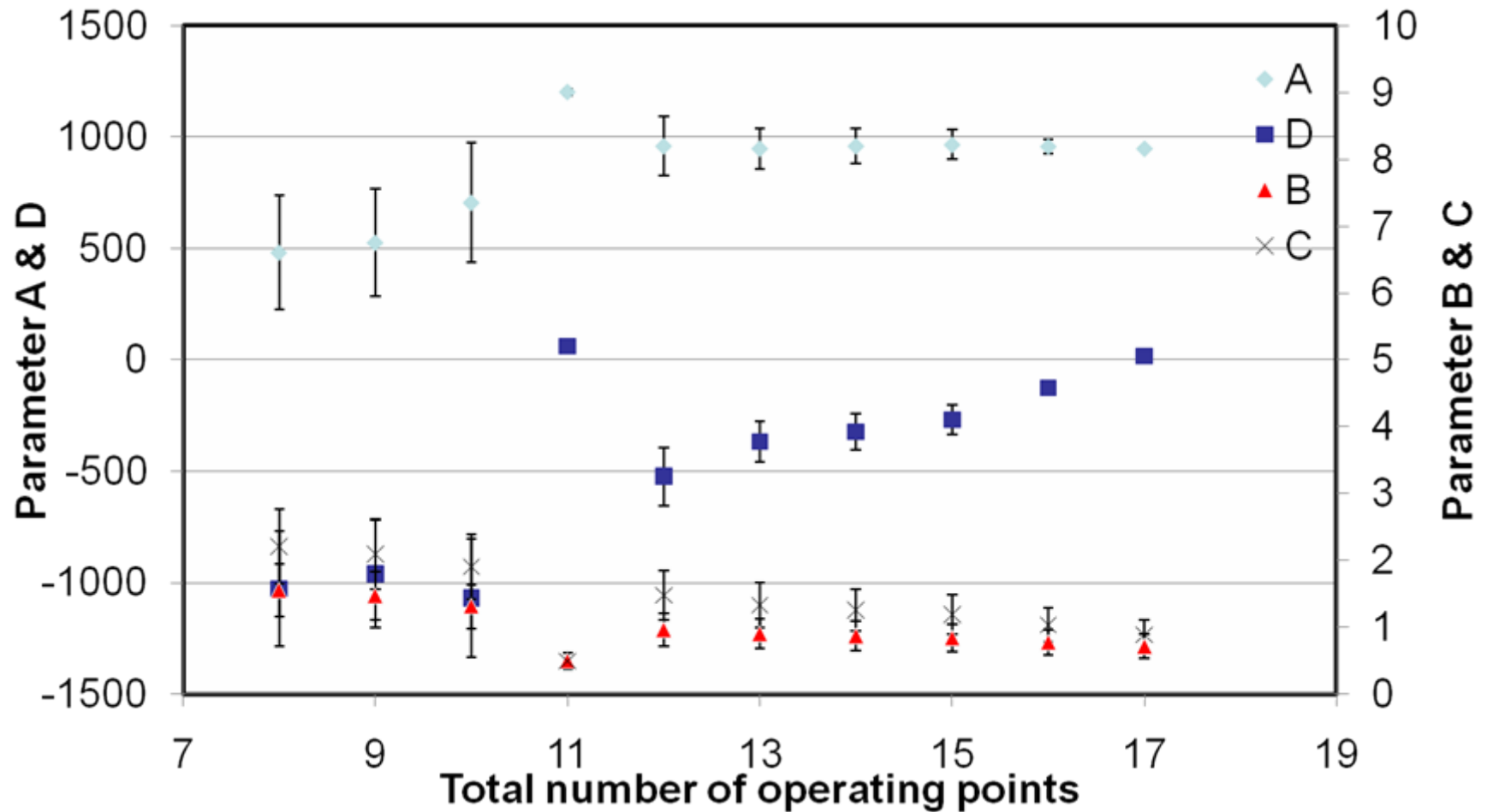
Optimised parameters A, B, C, D,
against database of
503 operating points from 7 engines



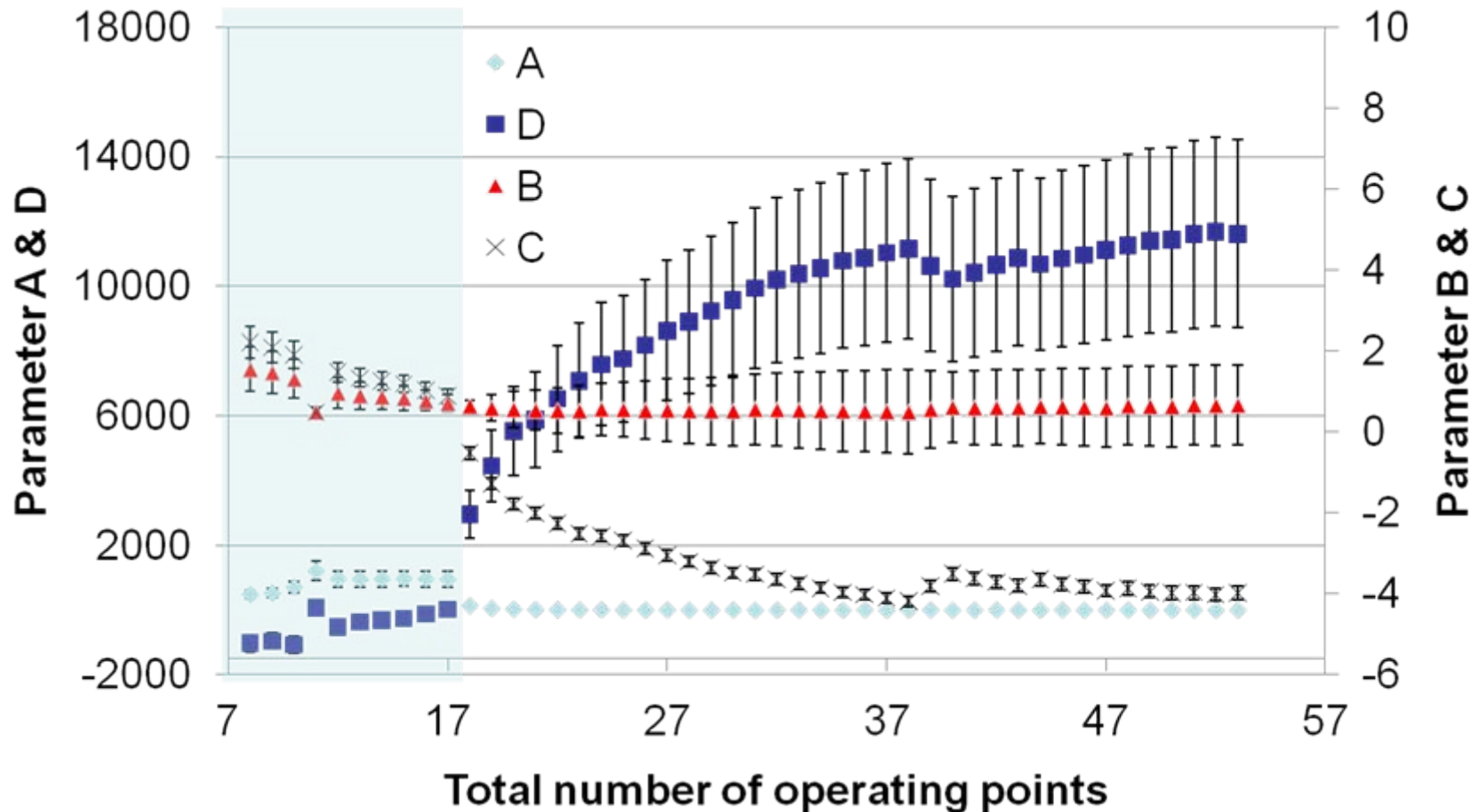
Example engine



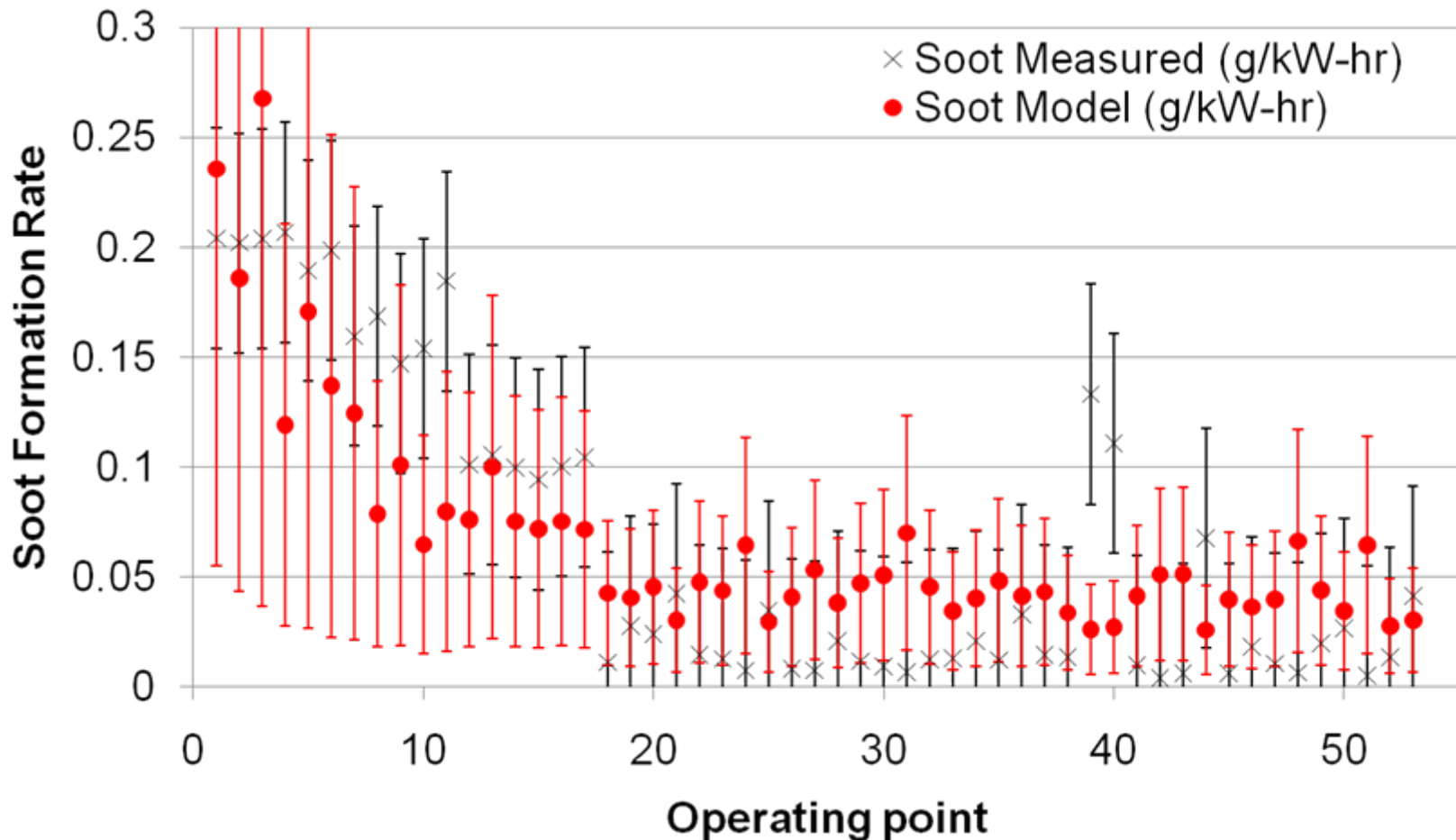
Parameter optimisation



Add data from second engine



Add data from second engine



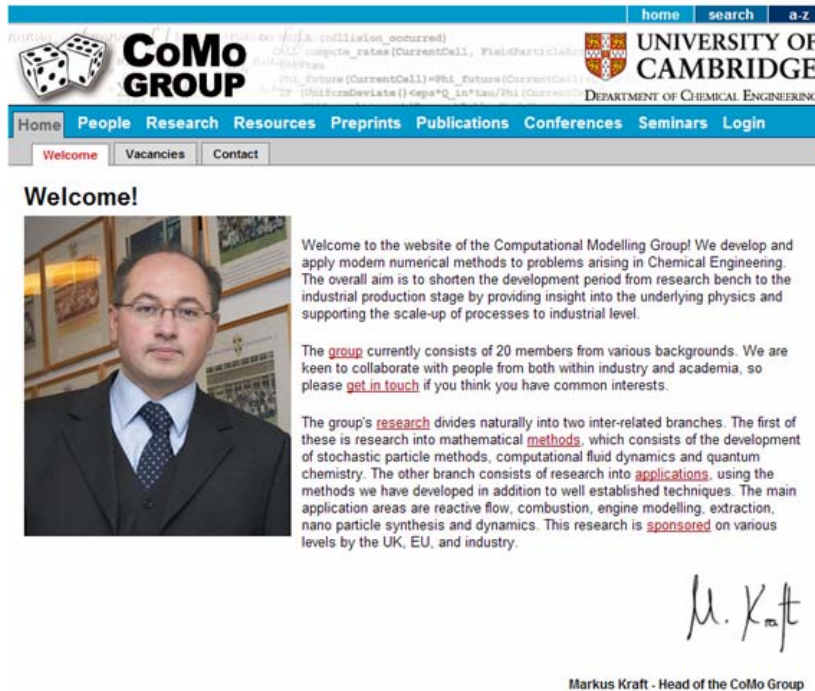
Summary

- Initial results of detailed soot modelling in a DISI engine have been presented, though, with room for improvement.
- A Process Informatics based methodology has been proposed for robust engine model development.
- A standardised, machine-readable format, engineML, has been presented.
- Optimisation results including model parameter and experimental uncertainties have been presented for an empirical diesel soot model.



Thank you!

Please visit our website:



The screenshot shows the homepage of the CoMo Group at the University of Cambridge. The header includes the CoMo Group logo (two dice) and the text 'CoMo GROUP' and 'UNIVERSITY OF CAMBRIDGE DEPARTMENT OF CHEMICAL ENGINEERING'. A navigation menu lists 'Home', 'People', 'Research', 'Resources', 'Preprints', 'Publications', 'Conferences', 'Seminars', and 'Login'. Below the menu, there are buttons for 'Welcome', 'Vacancies', and 'Contact'. The main content area features a 'Welcome!' heading, a portrait of Markus Kraft, and three paragraphs of text describing the group's mission, membership, and research areas. A handwritten signature of Markus Kraft is visible below the text.

Welcome!

Welcome to the website of the Computational Modelling Group! We develop and apply modern numerical methods to problems arising in Chemical Engineering. The overall aim is to shorten the development period from research bench to the industrial production stage by providing insight into the underlying physics and supporting the scale-up of processes to industrial level.

The [group](#) currently consists of 20 members from various backgrounds. We are keen to collaborate with people from both within industry and academia, so please [get in touch](#) if you think you have common interests.

The group's [research](#) divides naturally into two inter-related branches. The first of these is research into mathematical [methods](#), which consists of the development of stochastic particle methods, computational fluid dynamics and quantum chemistry. The other branch consists of research into [applications](#), using the methods we have developed in addition to well established techniques. The main application areas are reactive flow, combustion, engine modelling, extraction, nano particle synthesis and dynamics. This research is [sponsored](#) on various levels by the UK, EU, and industry.

M. Kraft

Markus Kraft - Head of the CoMo Group

<http://como.cheng.cam.ac.uk>



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