14th ETH-Conference on Combustion Generated Nanoparticles
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Paper/Poster-Abstract Form

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Title: Modelling soot formation in a Direct Injection Spark Ignition engine

Abstract: (min. 300 – max. 500 words)

The abstracts for papers and posters must contain unpublished information on the research subject: background, investigation methods, results and conclusions. Graphs and references are very welcome. Acronyms should be avoided. Abstracts with < 300 words can not be considered.

In this work, the formation of soot in a Direct Injection Spark Ignition (DISI) engine is simulated using the Stochastic Reactor Model (SRM) engine code. Turbulent mixing, convective heat transfer, direct injection and flame propagation are accounted for. In order to simulate flame propagation, the cylinder is divided into an unburned, entrained and burned zone, with the rate of entrainment being governed by empirical equations but combustion modelled with chemical kinetics. The model contains a detailed chemical mechanism as well as a highly detailed soot formation model, however computation times are relatively short. The soot model provides information on the morphology and chemical composition of soot aggregates along with bulk quantities, including soot mass, number density, volume fraction and surface area. The model is first calibrated by simulating experimental data from a Gasoline Direct Injection (GDI) Spark Ignition (SI) engine. The model is then used to simulate experimental data from the literature, where the numbers, sizes and derived mass particulate emissions from a 1.83 L, 4-cylinder, 4 valve production DISI engine were measured in the exhaust gas. Experimental results from different injection and spark timings are compared with the model, which is capable of reproducing qualitative trends in aggregate size distribution and emissions.
Secondly, we use this example of DISI soot modelling in order to illustrate more generally what can be achieved with present modelling approaches and what the limitations are. We discuss the role experimental data plays in the process of building models and propose a standardised, systematic way of storing and processing data. We emphasise in particular the importance of accounting for uncertainties in measurements and model parameters. We then demonstrate how such an infrastructure can be applied to quantitatively assess an empirical soot model against a large experimental database, highlighting potential model shortcomings and outliers in the data.

Short CV of presenter:
Amit Bhave is presently a Fellow at Hughes Hall, Cambridge and an Affiliate Research Fellow at the CoMo Group, Department of Chemical Engineering & Biotechnology, Cambridge. Amit's research interests include numerical modelling, low-emission combustion engines, chemical reactor design, and technology commercialisation. Amit completed his PhD at Cambridge and has Bachelors and Masters Degrees in Chemical Engineering. As the CEO, he manages cmcl innovations, a technology-intensive SME serving the automotive, chemical/materials and energy industries.

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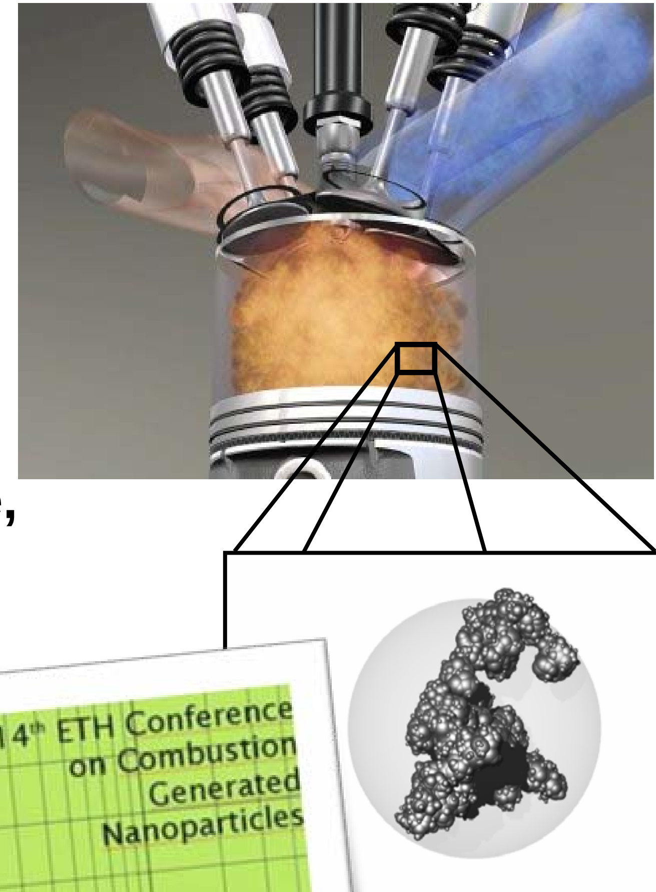
Modelling soot formation in direct injection SI engines



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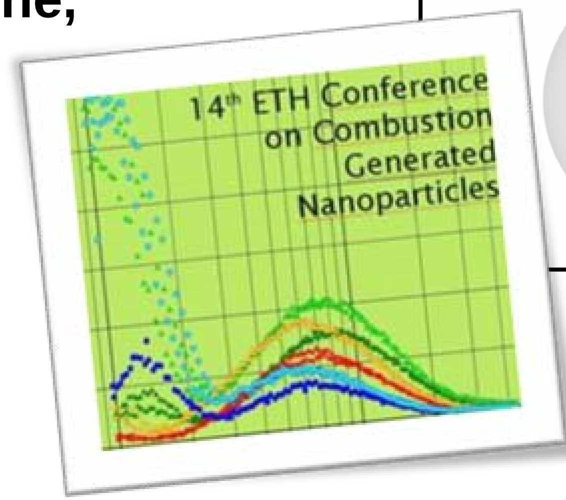

02 Aug. 2010

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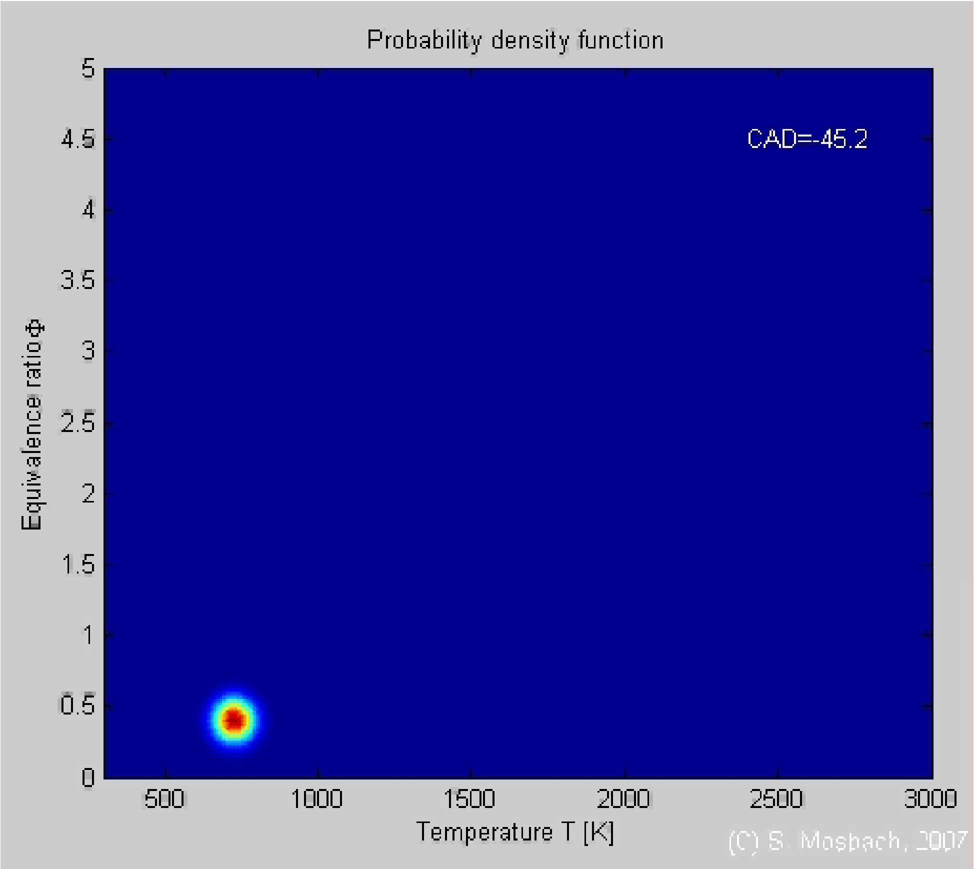
Stochastic Reactor Model (SRM)

- Closed-volume in-cylinder processes.
- Turbulent mixing, heat transfer, direct injection, piston movement, spark ignition, soot formation.
- Detailed chemical model - 208 species, 1002 reactions



Test case:
PFI and DI at 40 CAD BTDC

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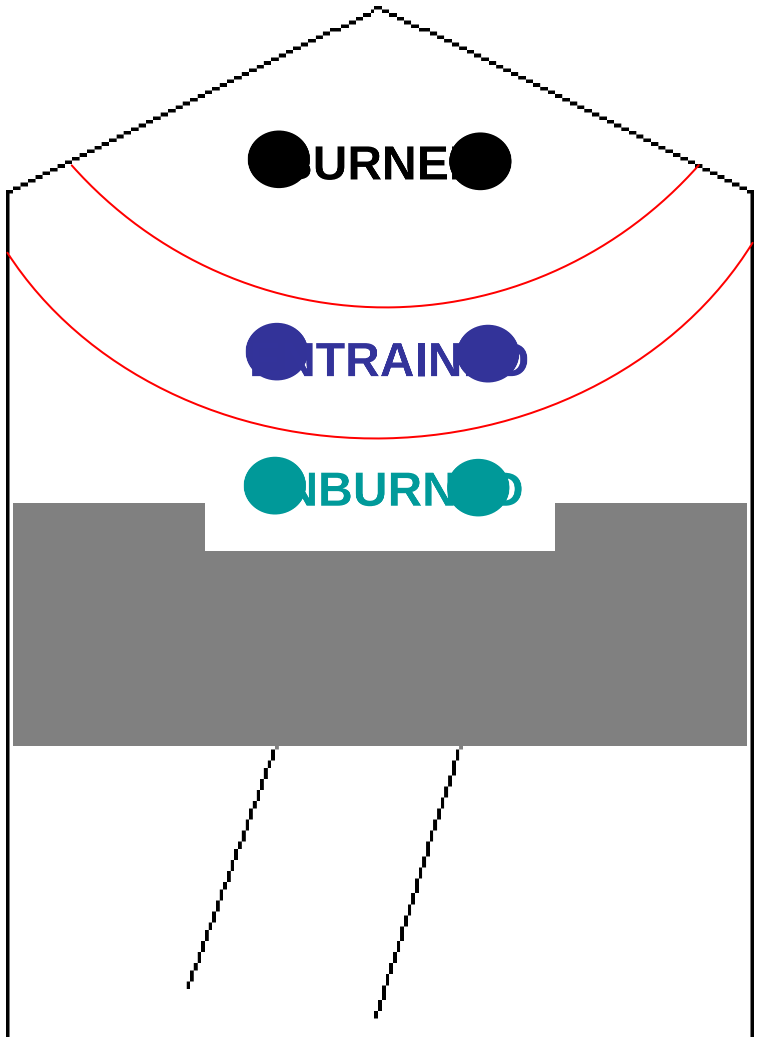
SRM-SI



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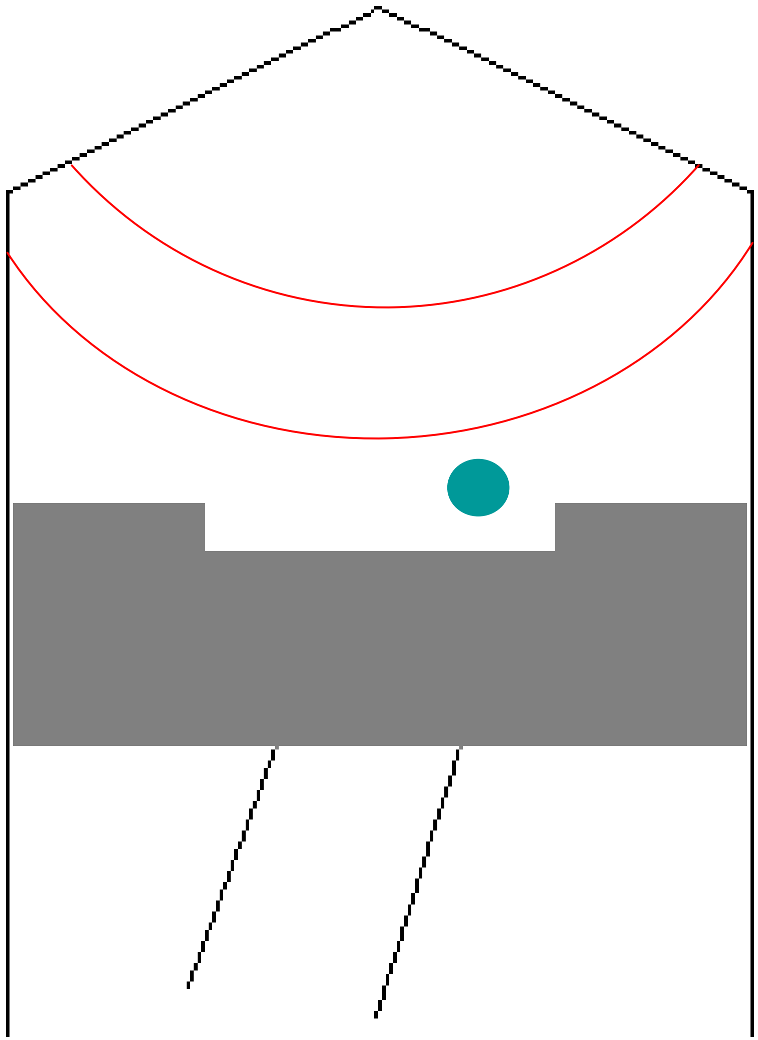
SI model



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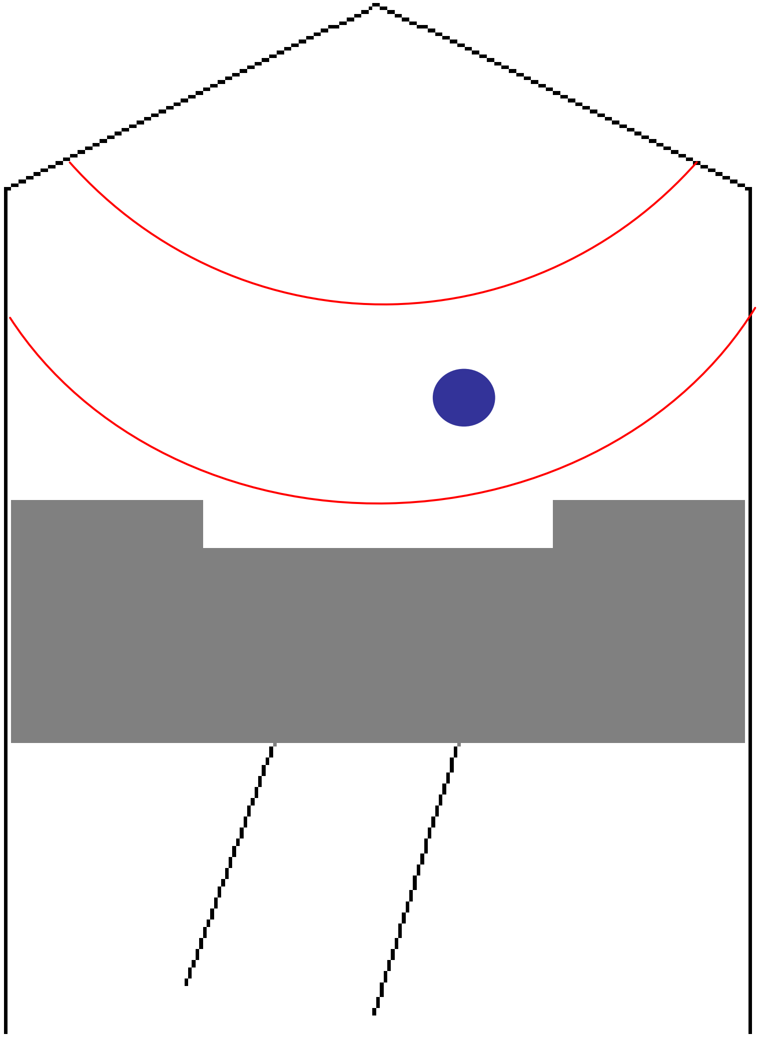
SI model



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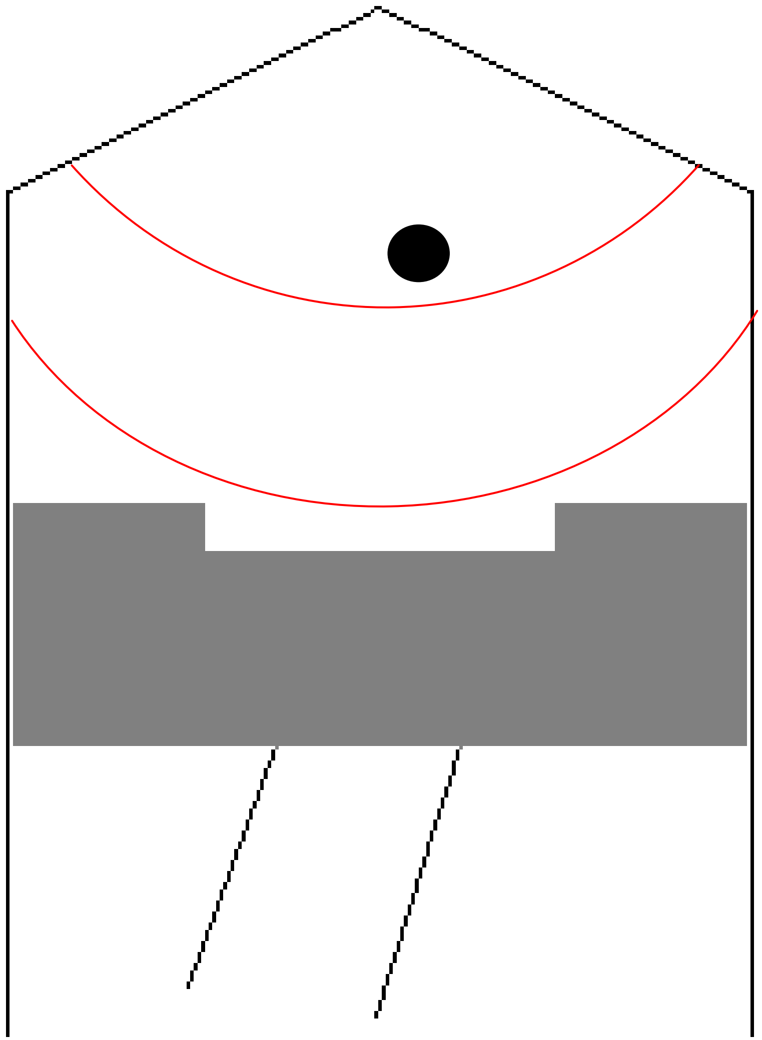
SI model



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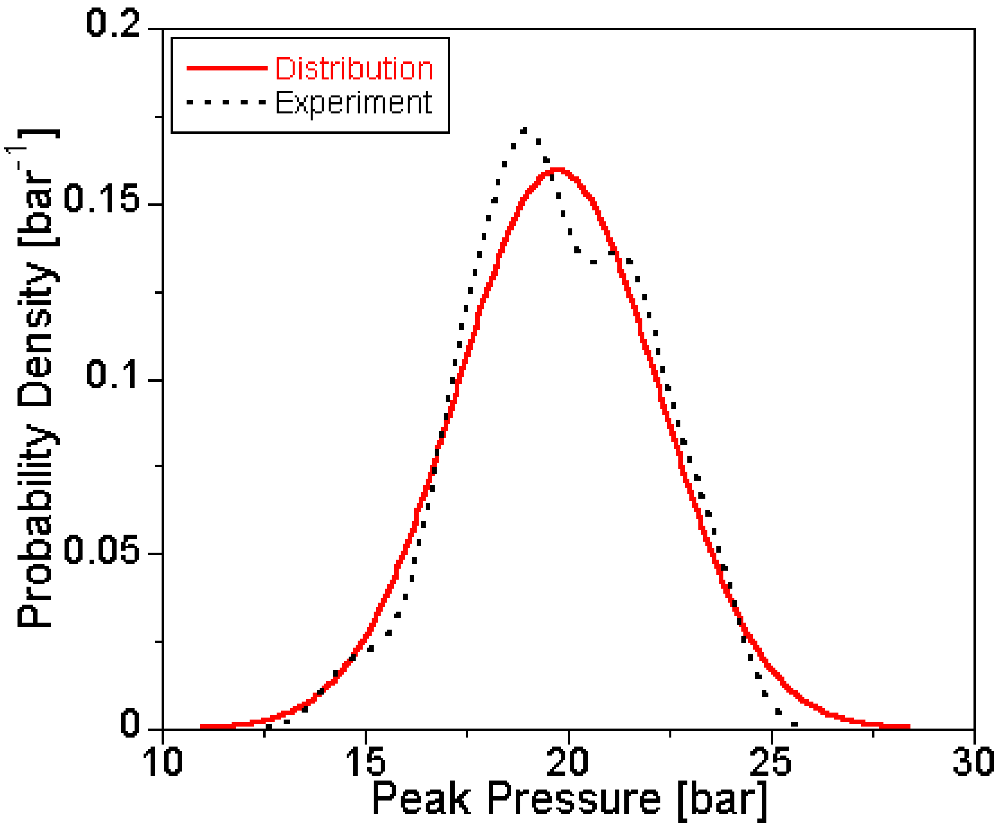
SI engine CCV

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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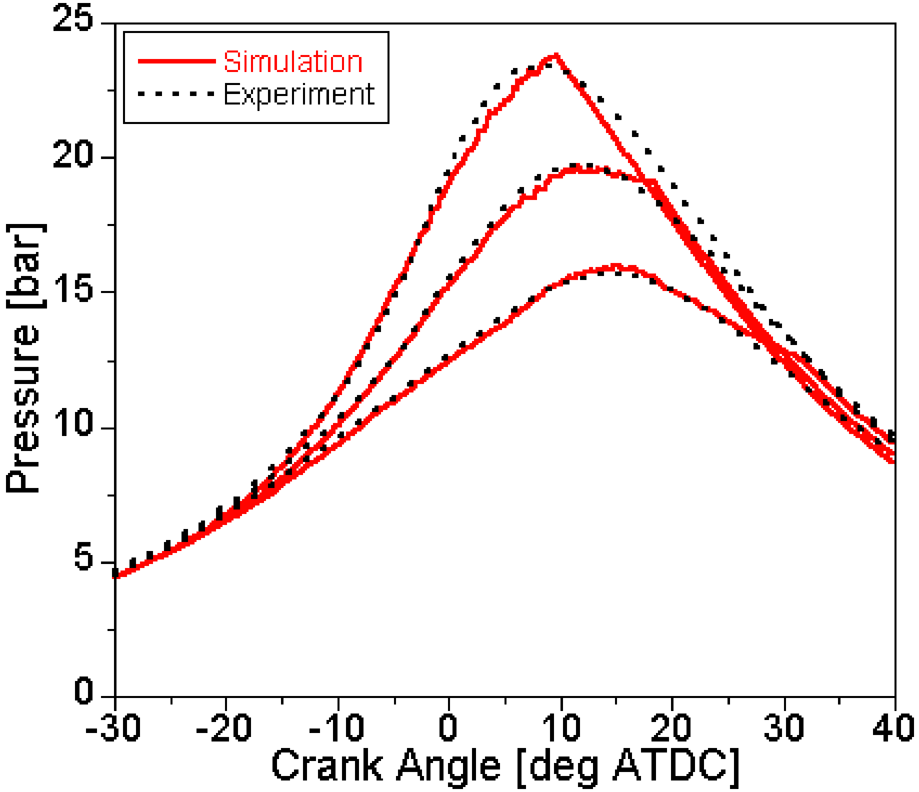
SI model calibration



- Characteristic flame speed obtained from:

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

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

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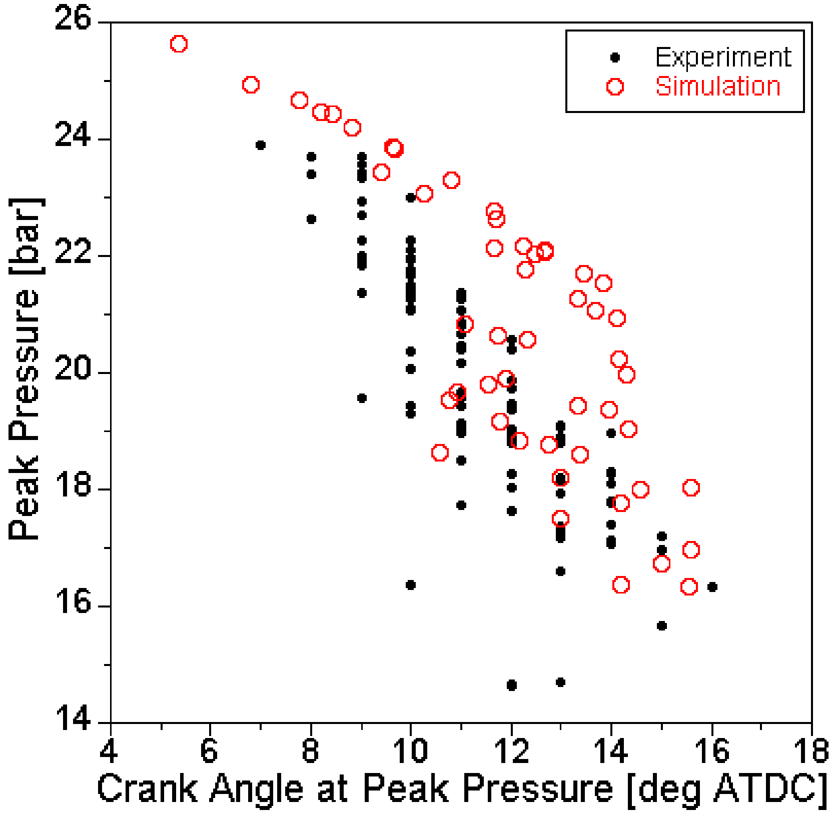
Multi-cycle SI simulation



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

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DISI engine

Image from www.engineforall.com

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

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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, Φ=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

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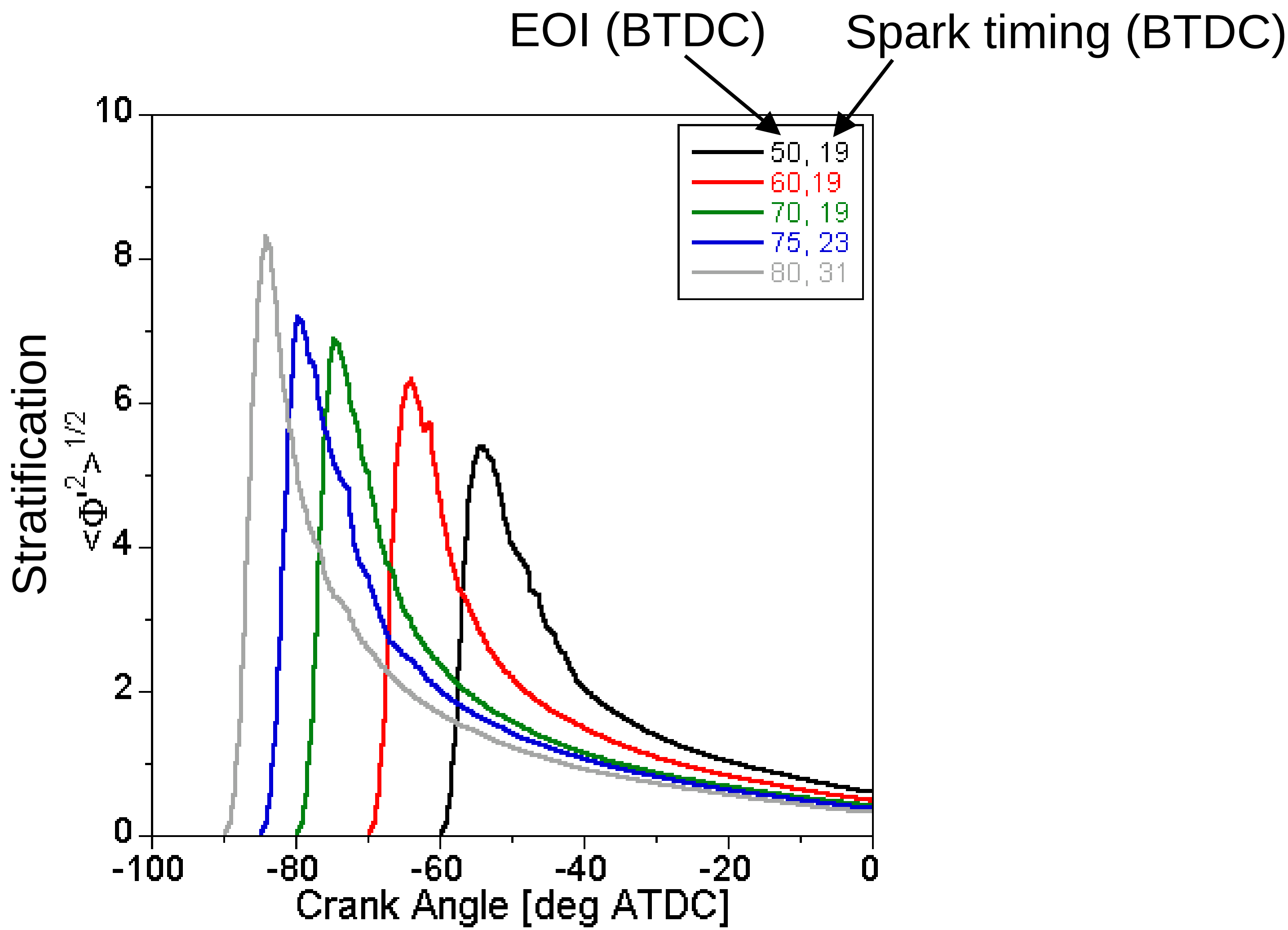
DISI engine simulation results



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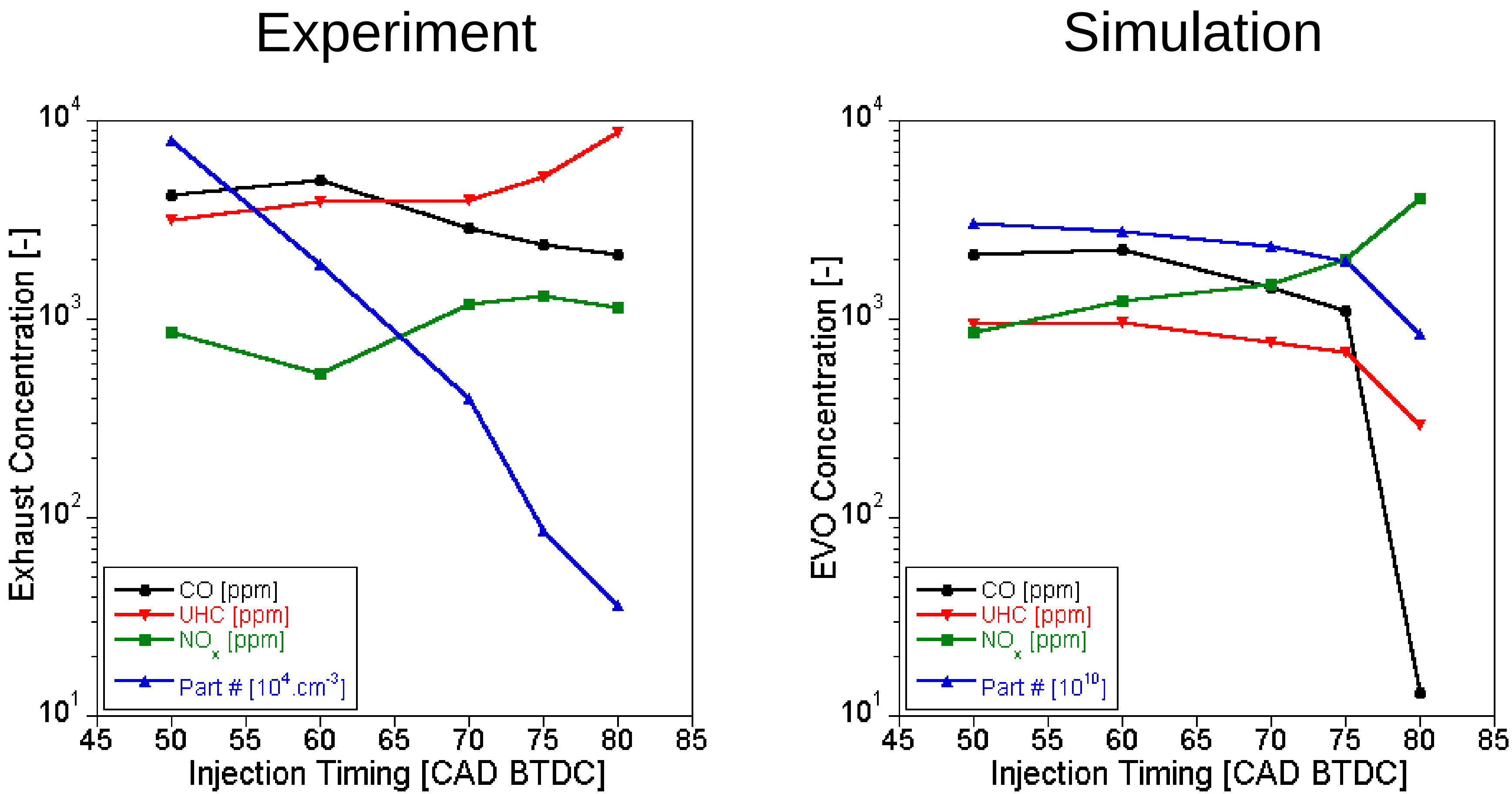
DISI engine emissions



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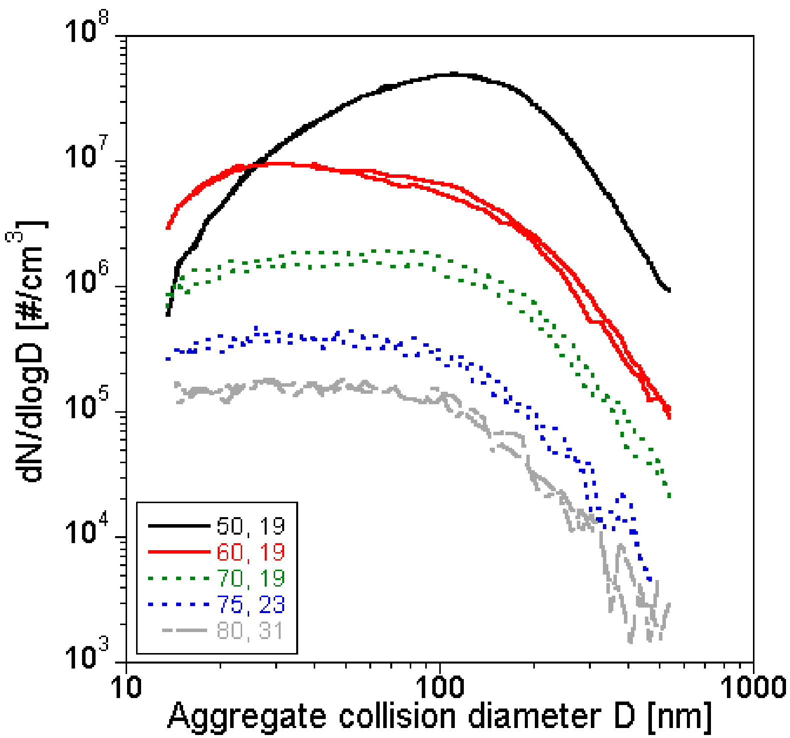
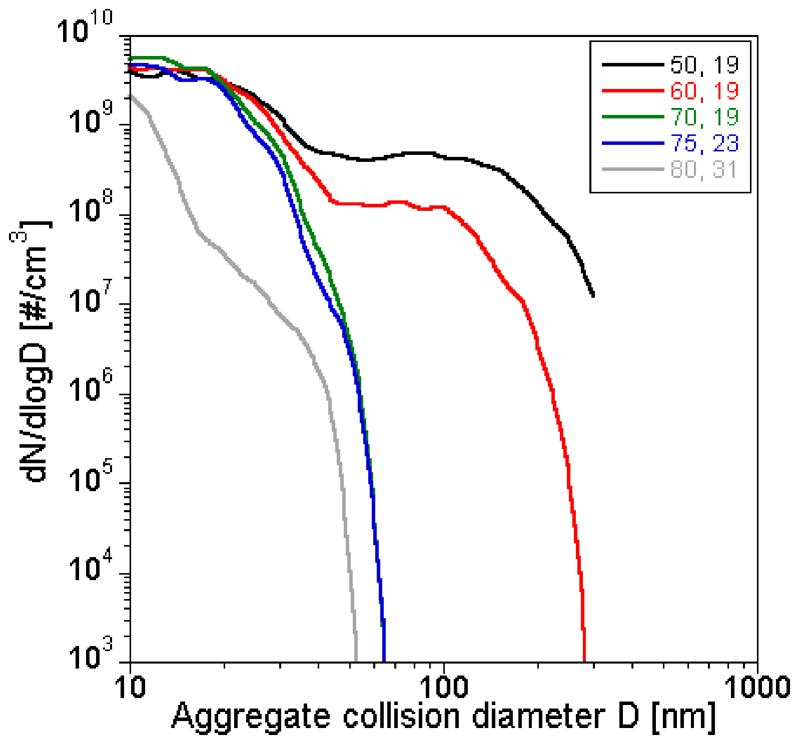
Particle size distributions

Experiment



Simulation



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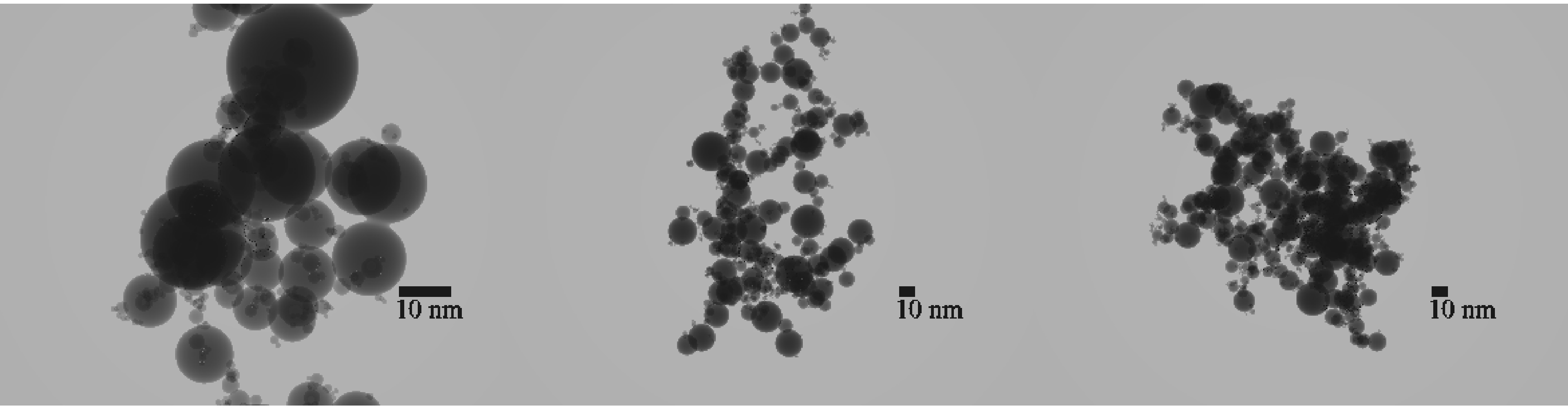
Soot in DISI engine

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

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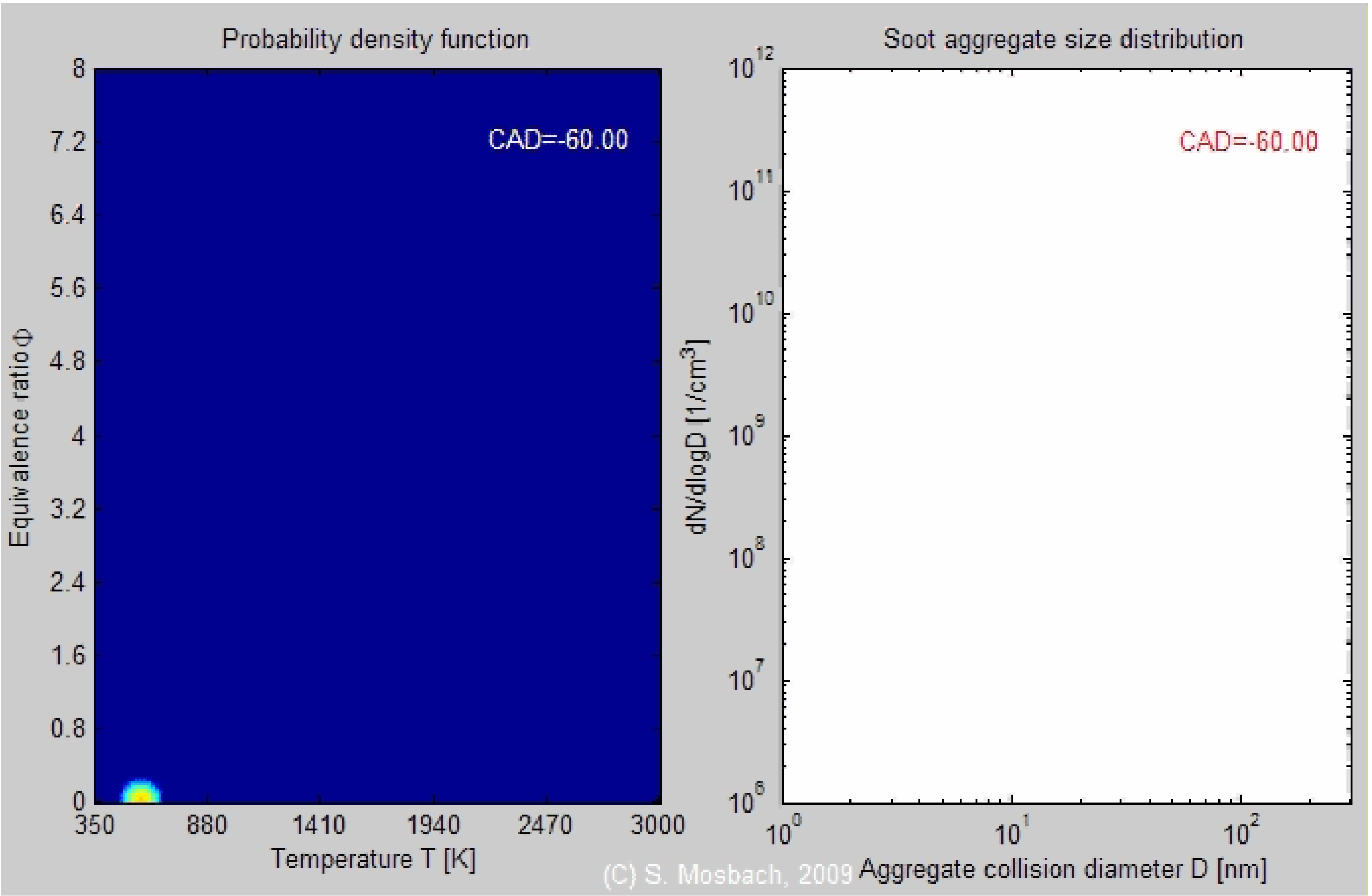
Temporal evolution (late injection)



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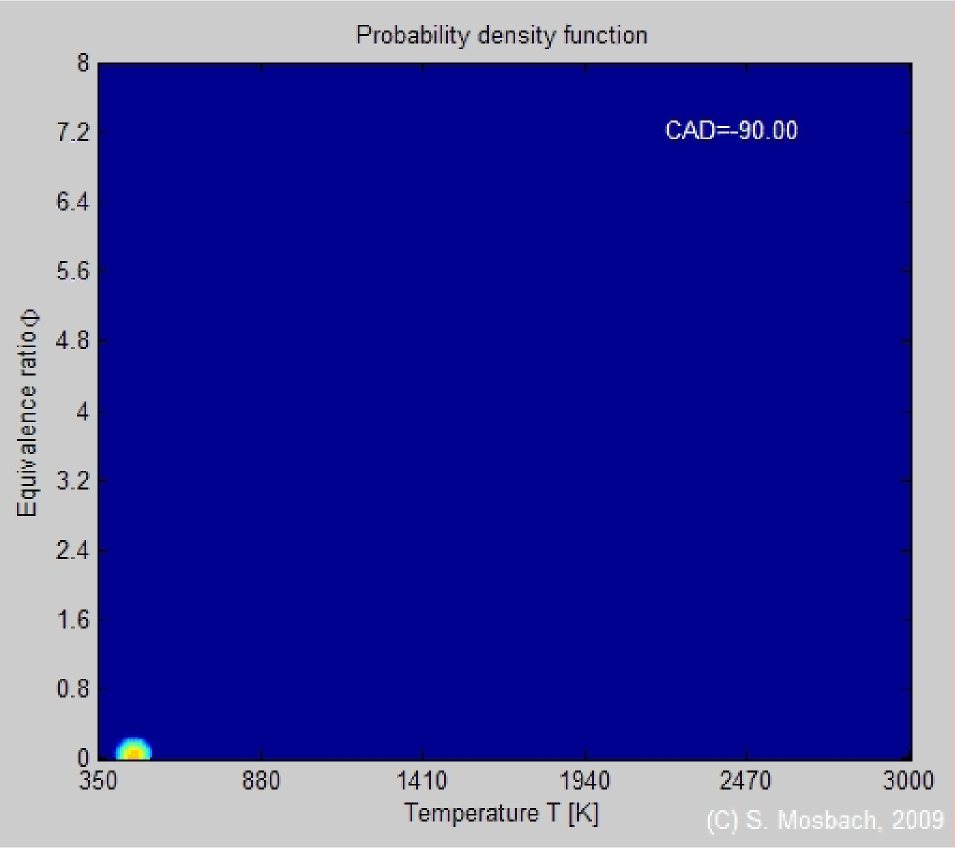
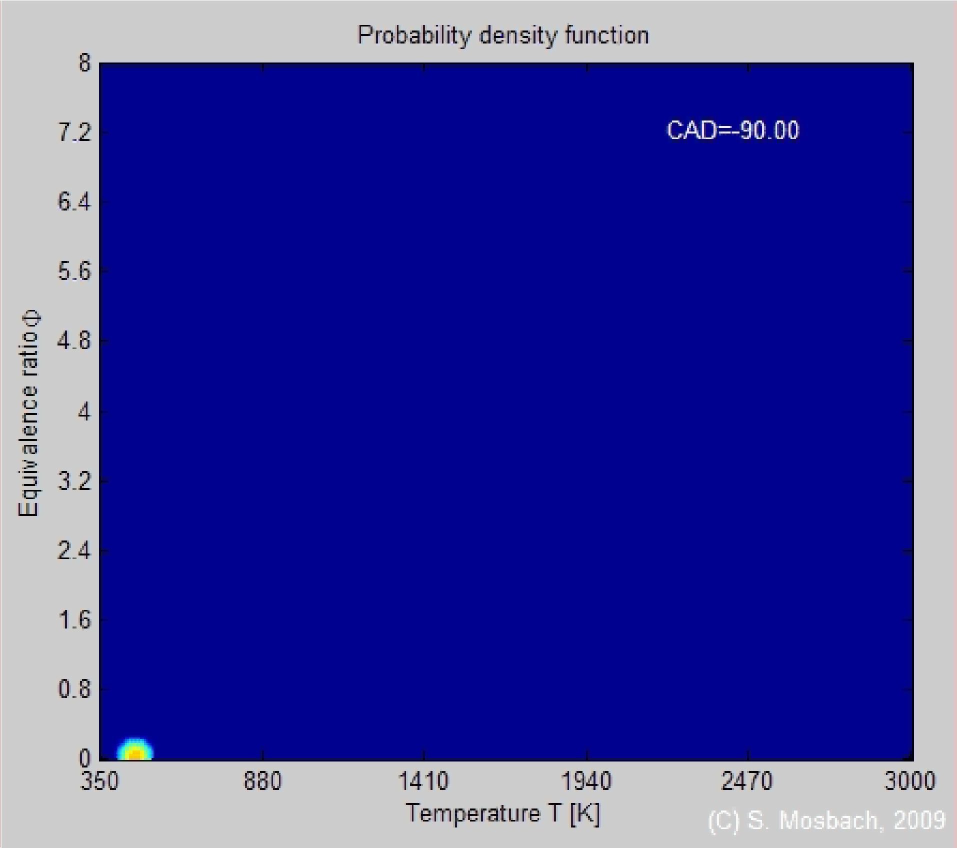
Comparison early/late injection

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

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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

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A data model: engineML

Consistent format

- point data (e.g. rpm, CO, u_l)
- 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"

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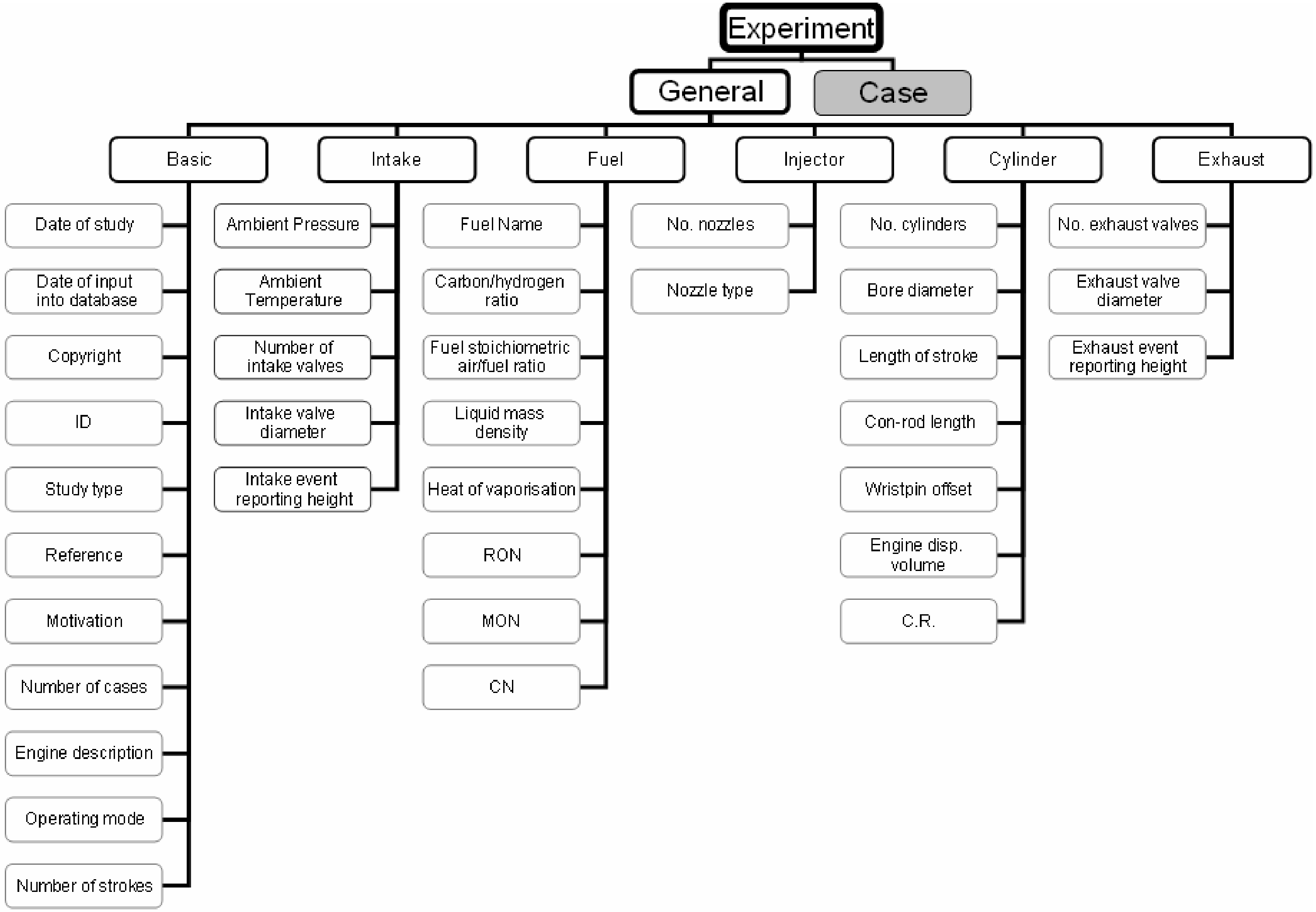
General data



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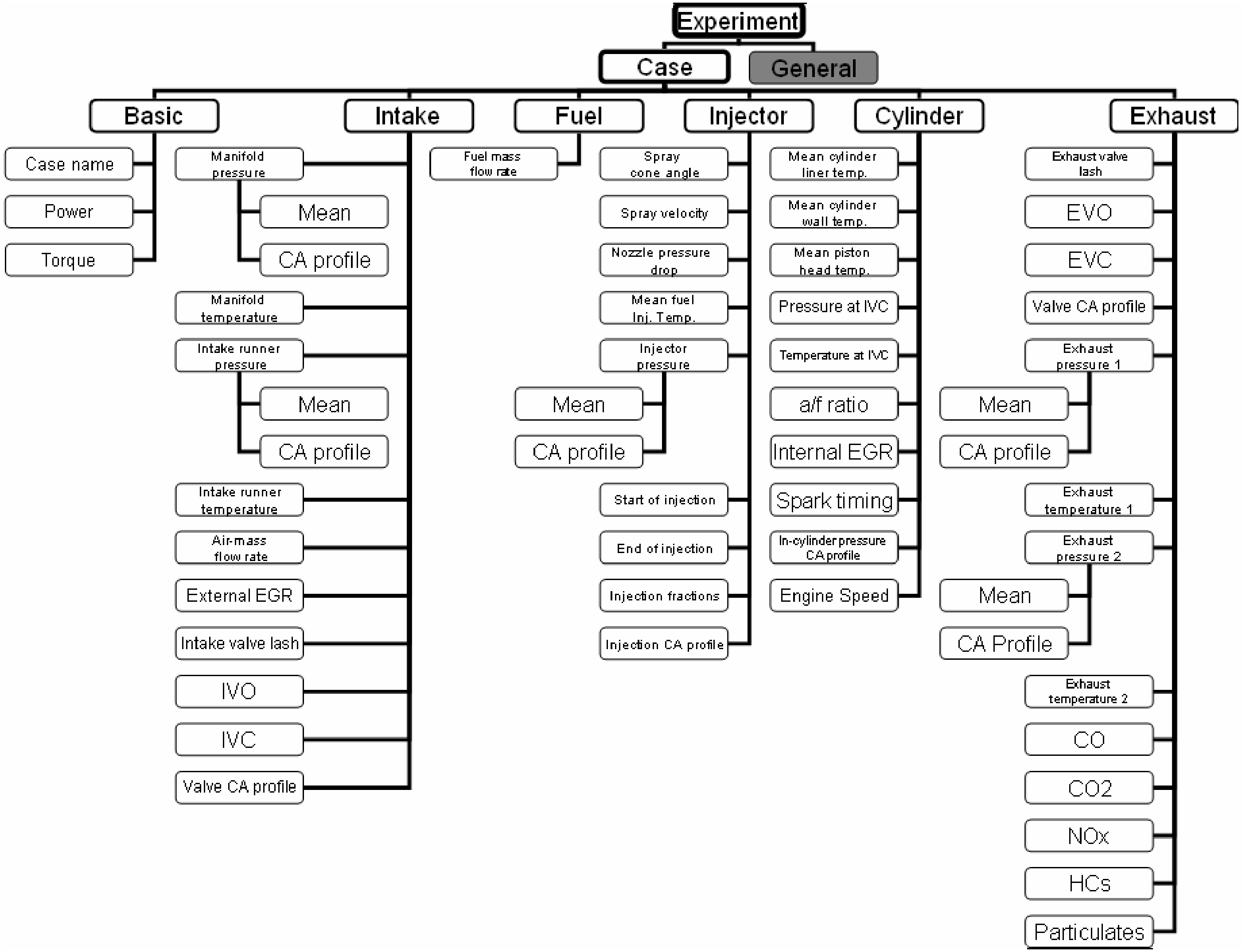
Case data



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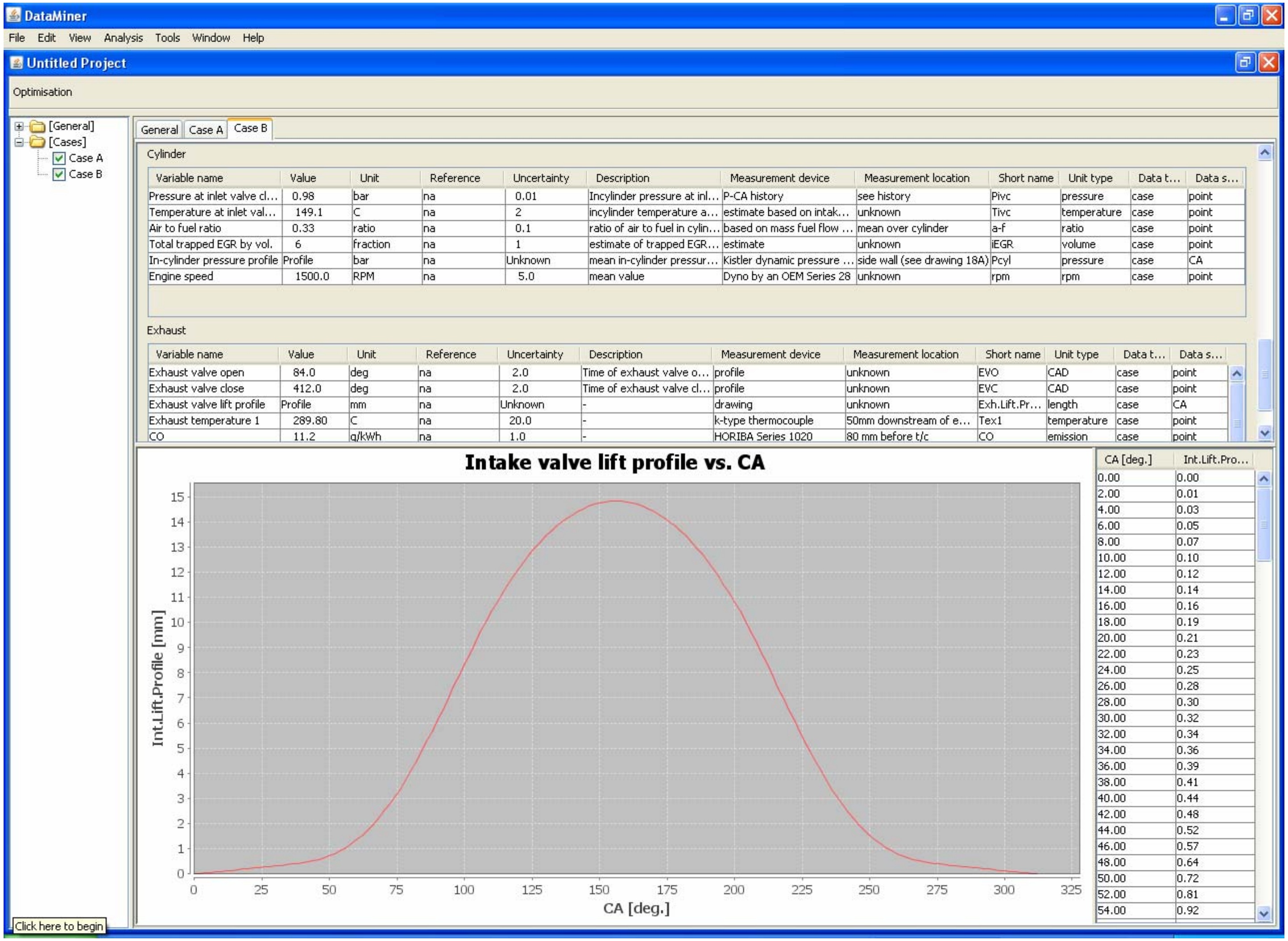
Data visualisation



Cylinder

Variable name	Value	Unit	Reference	Uncertainty	Description	Measurement device	Measurement location	Short name	Unit type	Data t...	Data s...
Pressure at inlet valve cl...	0.98	bar	na	0.01	Incylinder pressure at inl...	P-CA history	see history	Pivc	pressure	case	point
Temperature at inlet val...	149.1	C	na	2	incylinder temperature a...	estimate based on intak...	unknown	Tivc	temperature	case	point
Air to fuel ratio	0.33	ratio	na	0.1	ratio of air to fuel in cylin...	based on mass fuel flow ...	mean over cylinder	a-f	ratio	case	point
Total trapped EGR by vol.	6	fraction	na	1	estimate of trapped EGR...	estimate	unknown	iEGR	volume	case	point
In-cylinder pressure profile	Profile	bar	na	Unknown	mean in-cylinder pressur...	Kistler dynamic pressure ...	side wall (see drawing 18A)	Pcyl	pressure	case	CA
Engine speed	1500.0	RPM	na	5.0	mean value	Dyno by an OEM Series 28	unknown	rpm	rpm	case	point

Exhaust

Variable name	Value	Unit	Reference	Uncertainty	Description	Measurement device	Measurement location	Short name	Unit type	Data t...	Data s...
Exhaust valve open	84.0	deg	na	2.0	Time of exhaust valve o...	profile	unknown	EVO	CAD	case	point
Exhaust valve close	412.0	deg	na	2.0	Time of exhaust valve cl...	profile	unknown	EVC	CAD	case	point
Exhaust valve lift profile	Profile	mm	na	Unknown	-	drawing	unknown	Exh.Lift.Pr...	length	case	CA
Exhaust temperature 1	289.80	C	na	20.0	-	k-type thermocouple	50mm downstream of e...	Tex1	temperature	case	point
CO	11.2	g/kWh	na	1.0	-	HORIBA Series 1020	80 mm before t/c	CO	emission	case	point

CA [deg.]	Int.Lift.Pro...
0.00	0.00
2.00	0.01
4.00	0.03
6.00	0.05
8.00	0.07
10.00	0.10
12.00	0.12
14.00	0.14
16.00	0.16
18.00	0.19
20.00	0.21
22.00	0.23
24.00	0.25
26.00	0.28
28.00	0.30
30.00	0.32
32.00	0.34
34.00	0.36
36.00	0.39
38.00	0.41
40.00	0.44
42.00	0.48
44.00	0.52
46.00	0.57
48.00	0.64
50.00	0.72
52.00	0.81
54.00	0.92

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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

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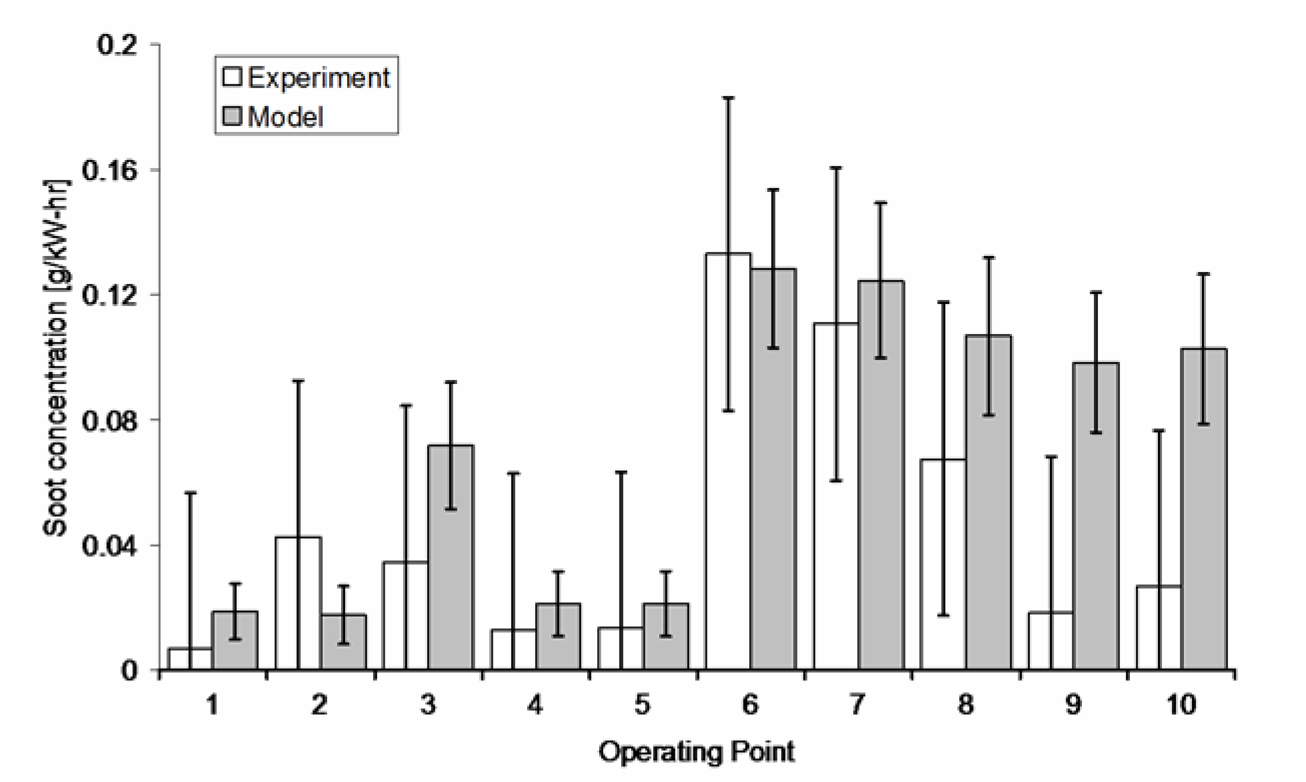
Application: Diesel soot

Empirical soot model (Plee):

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

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



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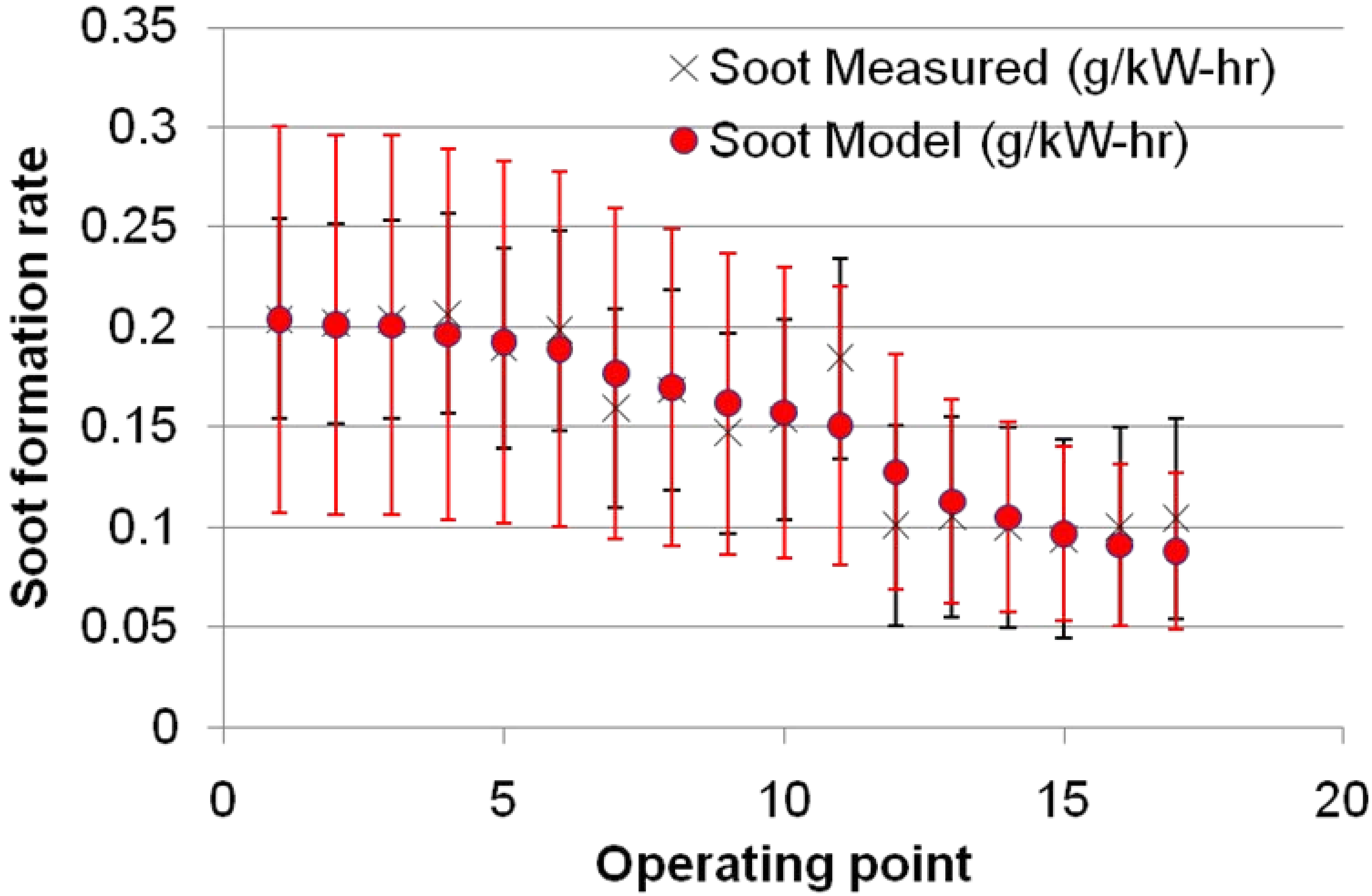
Example engine



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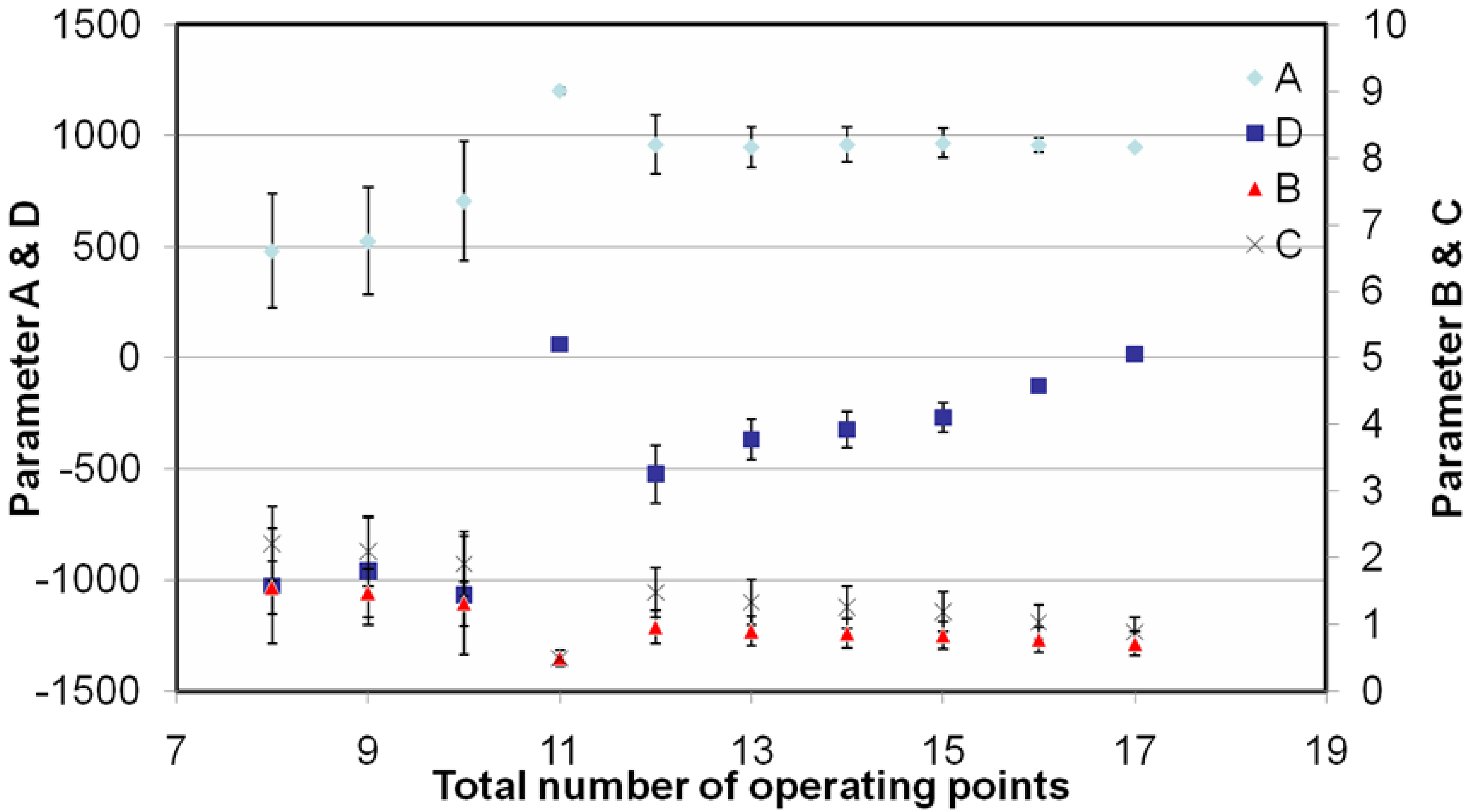
Parameter optimisation



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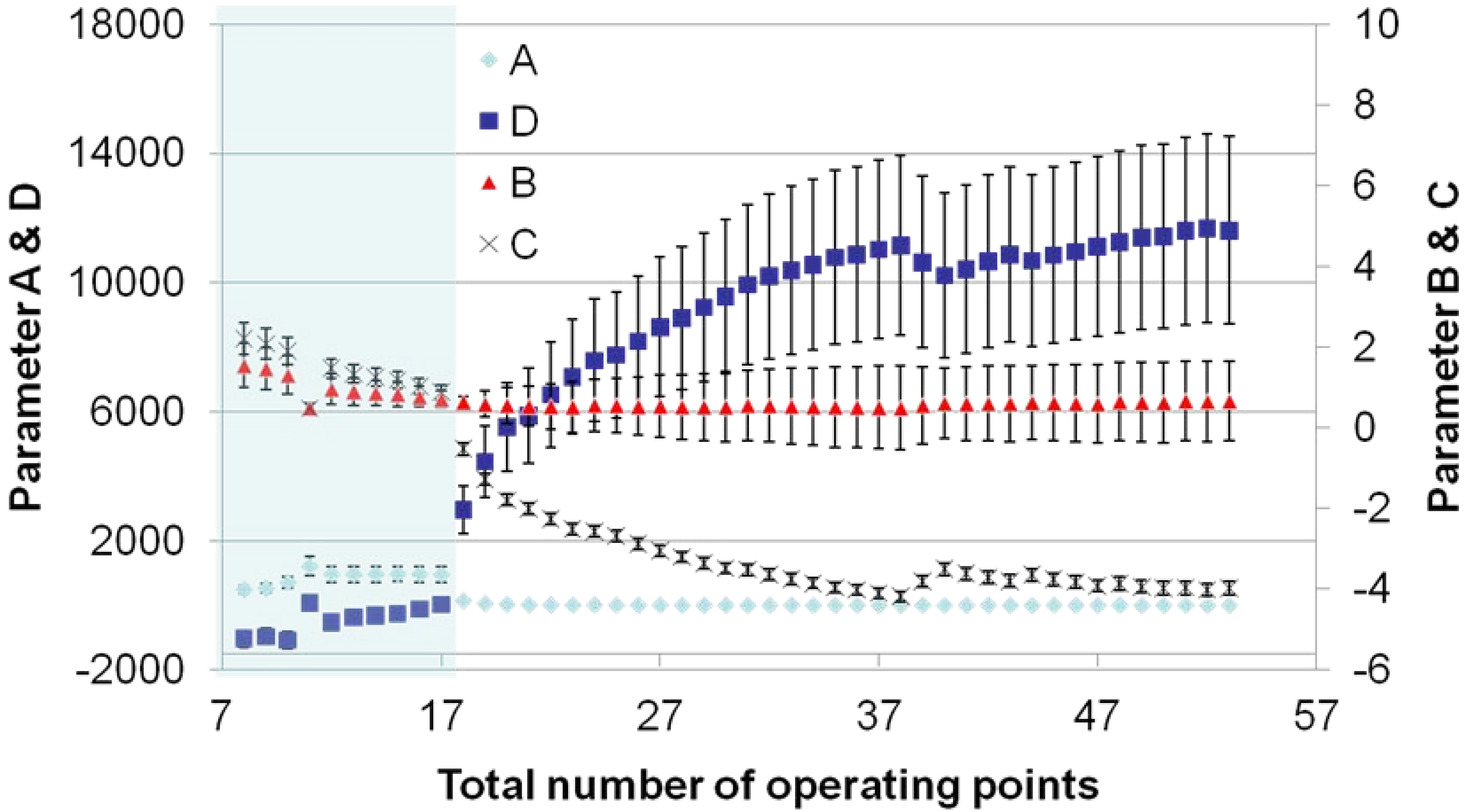
Add data from second engine



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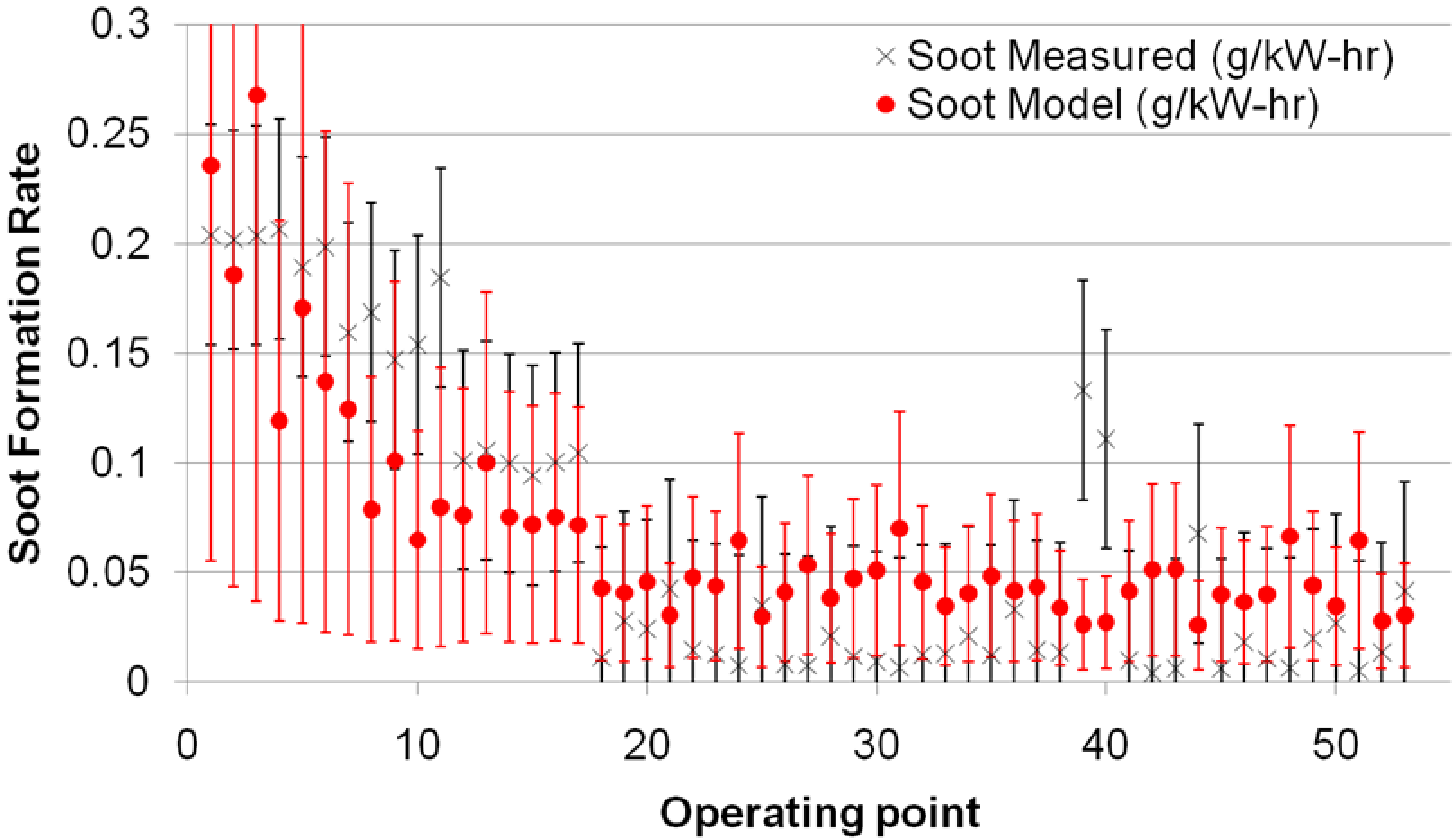

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Summary

- Results of detailed soot modelling in a DISI engine have been presented.
- 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.

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Thank you!

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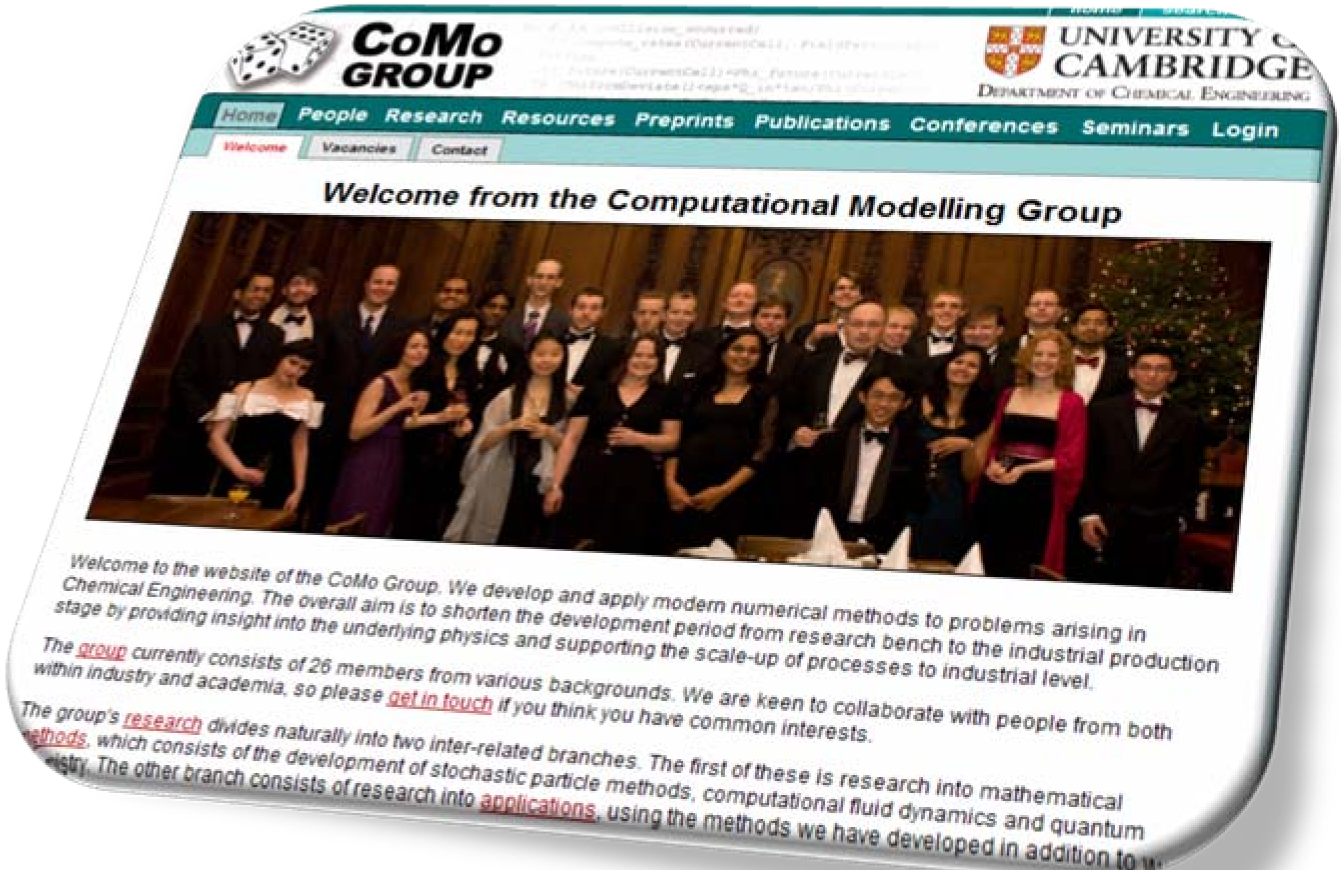

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Additional Slides

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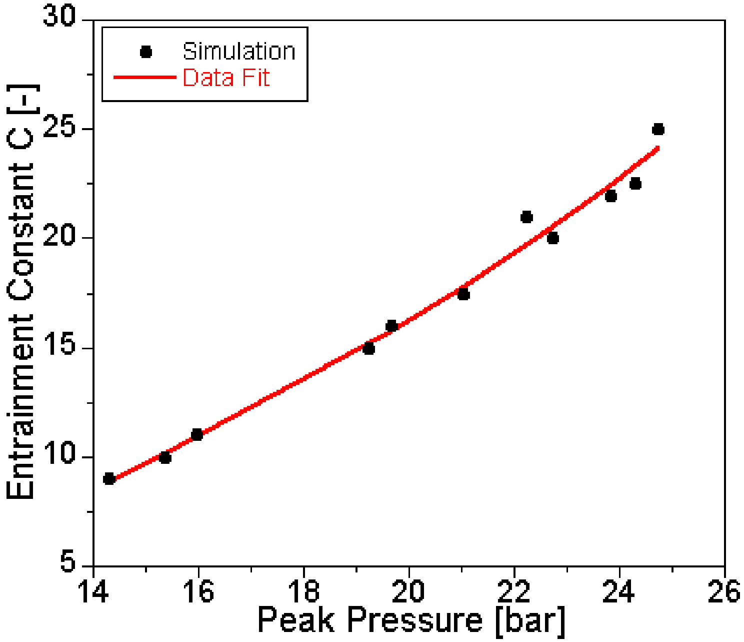
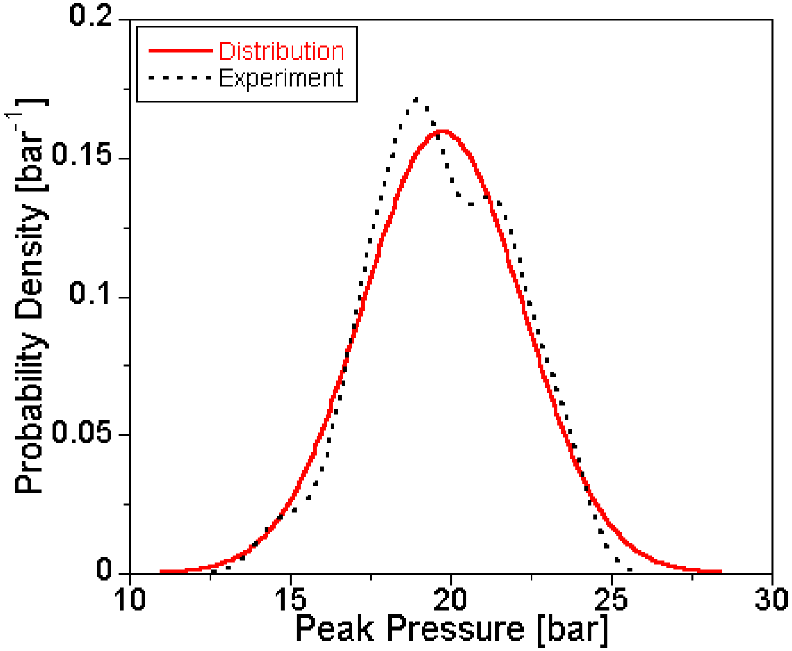
SI model calibration

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





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