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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The abstracts for papers and posters must contain unpublished information on the research subject: background, investigation methods, results and conclusions.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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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
SI model
SI model
SI model
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 cm³
CR: 12.0
Speed: 1500 RPM
Air/fuel equiv. ratio: 1.0
EGR: 28.8%

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Hopkinson Laboratory

DEPARTMENT OF
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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.
Multi-cycle SI simulation

- Model coupled to GT-Power for multi-cycle simulation.
- 50 simulated and 96 experimental cycles.
- NO\textsubscript{x} emissions:
  - 790 ppm simulation
  - 530 ppm experiment
DISI engine

• Late injection produces stratified mixture.

• Fuel rich regions close to spark gap.
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.

<table>
<thead>
<tr>
<th>Case</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>EOI [CAD ATDC]</td>
<td>-50</td>
<td>-60</td>
<td>-70</td>
<td>-75</td>
<td>-80</td>
</tr>
</tbody>
</table>

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

| Cylinders | 4 |
| Bore [mm]  | 81.0 |
| Stroke [mm] | 89.0 |
| Disp. volume [cm$^3$/cyl] | 457.5 |
| Compression Ratio | 12 |
DISI engine simulation results

EOI (BTDC)  Spark timing (BTDC)

Stratification vs. Crank Angle [deg ATDC]

-100 -80 -60 -40 -20 0

Stratification

Crank Angle [deg ATDC]
DISI engine emissions

Experiment

Simulation

CO [ppm]
UHC [ppm]
NOx [ppm]
Part # [10^4 cm^3]

CO [ppm]
UHC [ppm]
NOx [ppm]
Part # [10^18]

Injection Timing [CAD BTDC]

Exhaust Concentration [\text{-}]

EVO Concentration [\text{-}]

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Particle size distributions

Experiment

Simulation

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Soot in DISI engine

<table>
<thead>
<tr>
<th>CAD [deg ATDC]</th>
<th>2.6</th>
<th>12.6</th>
<th>32.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. Primaries</td>
<td>492</td>
<td>1315</td>
<td>2083</td>
</tr>
<tr>
<td>Coll. Diam [nm]</td>
<td>70</td>
<td>108</td>
<td>137</td>
</tr>
</tbody>
</table>
Temporal evolution (late injection)
Comparison early/late injection

EOI -80 CAD ATDC
Spark -31 CAD ATDC

EOI -50 CAD ATDC
Spark -19 CAD ATDC
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

Experiment
- General
  - Basic
    - Date of study
    - Date of input into database
    - Copyright
    - ID
    - Study type
  - Intake
    - Intake valve diameter
    - Intake event reporting height
  - Fuel
    - Fuel name
    - Carbon hydrogen ratio
    - Fuel stoichiometric air fuel ratio
    - Liquid mass density
    - Heat of vaporization
  - Injector
    - No. nozzles
    - Nozzle type
  - Cylinder
    - No. cylinders
    - Bore diameter
    - Length of stroke
    - Con-rod length
    - Wristpin offset
    - Engine disp. volume
    - C.R.
  - Exhaust
    - No. exhaust valves
    - Exhaust valve diameter
    - Exhaust event reporting height

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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):

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

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

![Graph showing soot formation rate vs operating point. The graph includes data points for measured soot and model predicted soot.]

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Parameter optimisation

![Graph showing parameter optimisation results](image)
Add data from second engine
Add data from second engine
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.
Thank you!

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Additional Slides
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.