Case study on Selective catalytic reduction (SCR) performance improvement over legislative engine cycles using 1D simulation

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Agenda

- Objective
  - SCR model calibration work flow
  - Standalone SCR modelling
  - Model calibration steps
  - Prediction for legislative engine test cycles
  - Model application for catalyst light-off study
  - Closing remarks
- Summary
Objective

- SCR catalyst NO\textsubscript{X} conversion performance improvement over legislative steady state and transient engine test cycles within defined boundaries of optimisation parameters for heavy duty Diesel engine considering BS-VI emission norms
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SCR modeling workflow

- **SCR standalone model building:**
  Chemical kinetics from reference literature
  Basic geometric data from catalyst supplier

- **Experimental data acquisition:**
  Engine and synthetic gas bench test data

- **Model calibration using experimental data:**
  Storage modelling correction
  NO\(_x\) conversion modelling correction

- **Model prediction for legislative engine cycles:**
  Steady state (WHSC)
  Transient cycles (WHTC)

- **Model application for concept evaluation:**
  Variation of catalyst sizing,
  Catalyst light off study etc.
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SCR standalone model building approach

- Flexible and quick
- Quasi steady approach
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Model calibration: Literature data

Standalone SCR Model work based on literature data:

- Initial reaction kinetics from GT-suite examples
- Data from literature for Cu-Zeolite catalyst
- Reaction kinetics tuned
- Advanced statistical optimisation tools

Work presented in GT conference 2017, Pune, India
Active site density, Adsorption and Desorption rate constants are calibrated

Calibrated rate constants to be validated for NH$_3$ step feed on engine test bench
Model calibration: SGTB data - NO\textsubscript{X} Conversion

Test Conditions:
- GHSV = 84K
- ANR = 1
- NO\textsubscript{X} = 500 PPM
Model calibration: Engine test bed

<table>
<thead>
<tr>
<th>Engine specifications</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of cylinders</td>
<td></td>
</tr>
<tr>
<td>Category</td>
<td>Heavy duty Diesel</td>
</tr>
<tr>
<td>Target emission level</td>
<td>BS-VI</td>
</tr>
<tr>
<td>NO\textsubscript{x} control strategy</td>
<td>SCR only (No EGR)</td>
</tr>
<tr>
<td>Aftertreatment layout</td>
<td>DOC + cDPF + SCR</td>
</tr>
<tr>
<td>SCR volume (l)</td>
<td>~ 10</td>
</tr>
<tr>
<td>SCR catalyst</td>
<td>Cu-Zeolite</td>
</tr>
</tbody>
</table>

Model considerations:
- Standalone SCR model
- DPF out data mapped as inlet BC to SCR
- Uniform Urea decomposition
- NH\textsubscript{3} mapped as inlet BC

Test Engine layout

- Temperature
- Pressure
- NO, NO\textsubscript{2}, CO, HC, CO\textsubscript{2}
- O\textsubscript{2}, H\textsubscript{2}O
- Mass/Volume flow rate

- Temperature
- Pressure
- NO, NO\textsubscript{2}, CO, HC, CO\textsubscript{2}

- Temperature
- Pressure
- NO, NO\textsubscript{2}

- Temperature
- Pressure
- NO, NO\textsubscript{2}, O\textsubscript{2}, H\textsubscript{2}O
- NH\textsubscript{3}

- Temperature
- Pressure
- NO, NO\textsubscript{2}, O\textsubscript{2}, H\textsubscript{2}O
- NH\textsubscript{3}
Model calibration: Engine test data - steady state

- $T_{\text{SCR\,in}} = 367(\text{degC})$
- $SV = 24K(\text{h}^{-1})$

- NH$_3$ Storage modelling calibrated (step feed)
- NO$_x$ conversion reaction kinetics validated
- Entire engine operation window covered
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Model calibration: Engine test cycle

- Ramp mode engine test cycle
- Ammonia to $\text{NO}_x$ ratio of unity
- Transient test cycle
- Model captures transient trends
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Dosing starts when the Temperature crosses trigger temperature (~500 sec)

NO\textsubscript{X} conversion during light-off period is absent

Quick light-off is required for better cumulative NO\textsubscript{X} reduction efficiency
WHTC: Thermal management

- Conversion efficiency of the catalyst alone is not sufficient to meet targeted cycle emission

- With advanced light off temperature profile
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Closing remarks

- NH$_3$ dosing starts at threshold temperature
- Initial 500 seconds virtually no NO$_x$ conversion due to low temperature (no dosing)
- Reducing light off period significantly reduces cycle averaged NO$_x$ emission
- Thermal management demands hardware changes on engine
- Exhaust gas temperature could be controlled by following ways:
  - Exhaust throttle valve (ETV)
  - Air to fuel ratio control (Turbo charger)
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- Model built based on literature data is validated against physical test data
- Model calibration with NH$_3$ step feed experiments performed on engine test bed
- Model prediction is validated for transient test cycle operation
- Catalyst light-off study over transient test cycle using calibrated model
- Hardware change suggestion on physical engine to improve cycle average NO$_X$ conversion
Future work direction

- Performance comparison study of Zeolite and Vanadium catalysts over engine test cycles
- Modelling of Urea dosing system and NH$_3$ conversion efficiency
- Engine performance optimisation for improved thermal management and validation
- Predictive Engine model plus after-treatment modelling
- Test data validation for Vanadium catalyst
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THANK YOU!!