SCR

Current progress in Simulation of AdBlue Spray Preparation

AVL German Simulation Conference Ulm
16./17. Oktober 2018
1. Ensuring EAS performance
2. Wallfilm Chemistry
3. Runtime Considerations
4. Example Case
5. Outlook
Ensuring EAS performance

Application of 3D CFD to assess EAS performance
Problems addressed by 3D CFD simulation for AdBlue Spray Conditioning:

Quality of AdBlue spray conditioning
- Availability of NH3 at catalyst
- Uniformity of NH3

Reliability
- No depositions for given load point
- Spray impacting at catalyst
- How much AdBlue can safely be converted with given configuration

Front loading
- Selection of most suited injector
- Availability of “preparation margin” per load points → what raw emissions am I able to convert
Wallfilm chemistry

Solid Particle Chemistry in Wallfilm
SCR Depositions
Wallfilm chemistry

Kinetic reaction mechanism of urea decomposition.

States of aggregation:
(s): solid,
(m): molten,
(g): gaseous,
(l): liquid/dissolved.

Kinetic modeling of urea decomposition based on systematic thermogravimetric analyses of urea and its most important by-products, Brack et.al., Chemical Engineering Science 106 (2014) 1-8
Kinetic reaction mechanism of urea decomposition.

States of aggregation:

(s): solid,
(m): molten,
(g): gaseous,
(l): liquid/dissolved.

Solid products
SCR Depositions
Wallfilm chemistry

\[ T_{\text{gas}} = 110^\circ C \]

\[ T_{\text{gas}} = 225^\circ C \]

\[ T_{\text{gas}} = 450^\circ C \]

Solid film

\[ v_{\text{gas}} = 50 \text{m/s} \]

\[ m_{\text{AdBlue}} = 760 \text{g/h} \]
Runtime Considerations

The Gap: From Milliseconds to Minutes
(a) Variation Auslagerungstemperatur für eine Einwaage von 5mg Harnstoff
Abb. 3.14: Isotherme Zersetzung von Harnstoff (Experiment)

SCR Depositions
Runtime considerations
SCR Depositions Runtime considerations

Gas Flow
\[ \Delta t \approx 0.1 \text{ms} - \infty \]

Spray
\[ \Delta t < 1 \text{ms} \]

Solid
\[ \Delta t > 10 \text{ms} \]

Wallfilm
\[ \Delta t > 100 \text{ms} \]
SCR Depositions
Runtime considerations

With “best” settings and minimal numerical and modeling error currently 3s – 10s real time are feasible for simulation of load points.

\[ \Delta t < 1 \text{ms} \]
\[ \Delta t > 10 \text{ ms} \]
\[ \Delta t > 100 \text{ ms} \]
SCR Depositions
Runtime considerations

- Full simulation of 1\textsuperscript{st} injection
  - Detection of all droplets hitting walls
  - Averaging all sources
- Replay for all following injections:
  - Droplets appear at wall
  - Impinged droplets are deleted
  - All spray sources at wall are correctly calculated
Simulation complexity can be reduced by ~10x without changing wallfilm result resolution too much. Available in AVL FIRE v2018.
Example Case

Application of Deposition Simulation
**Randbedingungen Abgas/Wände**

**Aufbau Versuchsträger**

- Dosiermodul
- Heißgas
- DOC
- SDPF

**Wandmodellierung „Thin Wall“**

**Settings Thin Wall:**

- $\rho = 7830 \, \text{kg/m}^3$
- $h = 10 \, \text{W/m}^2\text{K}$
- $k = 52 \, \text{W/mK}$
- $c_p = 4,7 \, \text{J/kgK}$ (künstlich reduziert)

- DOC/SDPF isothermisch

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Thon, Per: "CFD-basierte Bewertung von Ablagerungsrisiken in einem motornahen Abgasreinigungskonzept", AVL AST Simulation Conference, München 2016
SCR Depositions

Example Case

Wallfilm thickness

Temperature

0µm – 300µm

100°C – 200°C
SCR Depositions
Example Case

Wallfilm thickness

Deposition thickness

0µm – 300µm

0µm – 200µm
SCR Depositions Example Case

Deposition thickness

0µm – 200µm

- Liquid + solid film
- Solid film
- Average wall temperature

~11g/h
### SCR Depositions

#### Example Case

- **Simulated solid deposition after 10 min**

**Total Runtime:**
- 600s/13dWCT/72CPU
- ~46s/dWCT/72CPU (@2.4GHz)
- 10s/dWCT/16CPU (@3.2GHz)

**Achieved project runtimes:**
- EAS model, 4.5mn cells:
  - 10s/dWCT/100CPU (@2.4GHz)
  \[ \rightarrow \] 1min/6dWCT
Outlook, Conclusions
Outlook
Transient Driving Cycle Simulation 3D → 1D

Simulation Workflow

CFD – characteristic OP simulation

Data transfer to 1D simulation model

1D transient driving cycle(s) simulation

Liquid mass injected (g)

Total film mass (g)

Liquid mass evaporated (g)

220_high

0

0.5

1

1.5

2

2.5

Time (s)

Liquid mass injected (g)

0 2 4 6 8 10

Time (s)

Liquid mass injected (g)

Injector mass flux

Mass flux

Temperatures

Mean Temperature - CAT2, SCR

Gas Temperature - Aftertreatment Boundary 1
Outlook

Transient Driving Cycle Simulation 3D → 1D

- HD exhaust line
- Simplified Geometry
- Artificial mixer geometry
- Fame Poly Mesh
- 4,200,000 cells
- w/o wall film reactions
- w/ wall film evaporation

DOC + DPF

Injection system

SCR

Wurzenberger, J.C., Nahtigal, A., Mitterfellner, T.: "1D/3D Simulation of Urea Dosing – Deposit Formation and NOx Reduction in Real Driving", SIA POWERTRAIN / ROUEN 2018
Outlook

Transient Driving Cycle Simulation 3D → 1D

<table>
<thead>
<tr>
<th>Gas Temp. [degC]</th>
<th>Mass Flow [kg/h]</th>
<th>Injected Mass [g/min]</th>
<th>No. of pulses</th>
</tr>
</thead>
<tbody>
<tr>
<td>220 Low</td>
<td>220</td>
<td>144</td>
<td>1.2</td>
</tr>
<tr>
<td>220 Mid</td>
<td>220</td>
<td>540</td>
<td>6</td>
</tr>
<tr>
<td>220 High</td>
<td>220</td>
<td>1080</td>
<td>13.5</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Gas Temp. [degC]</th>
<th>Mass Flow [kg/h]</th>
<th>Injected Mass [g/min]</th>
<th>No. of pulses</th>
</tr>
</thead>
<tbody>
<tr>
<td>280 Low</td>
<td>280</td>
<td>144</td>
<td>1.2</td>
</tr>
<tr>
<td>280 Mid</td>
<td>280</td>
<td>540</td>
<td>6</td>
</tr>
<tr>
<td>280 High</td>
<td>280</td>
<td>1440</td>
<td>15</td>
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<table>
<thead>
<tr>
<th>Gas Temp. [degC]</th>
<th>Mass Flow [kg/h]</th>
<th>Injected Mass [g/min]</th>
<th>No. of pulses</th>
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</thead>
<tbody>
<tr>
<td>360 Low</td>
<td>360</td>
<td>360</td>
<td>4.5</td>
</tr>
<tr>
<td>360 Mid</td>
<td>360</td>
<td>720</td>
<td>10.5</td>
</tr>
<tr>
<td>360 High</td>
<td>360</td>
<td>1260</td>
<td>15</td>
</tr>
</tbody>
</table>

Simulation matrix:
- 9 CFD cases selected from driving cycle
- Variation of gas temperature, mass flow and injected AdBlue

Simulation performance:
- 11s of physical time per day on 80 cores
- Frozen flow field/Database* technology enables a significant speed-up to conventional CFD

Outlook
Transient Driving Cycle Simulation 3D → 1D

Wall film thickness
Low  High

Urea dosing - animation

Wall Film Case 220 Low
Wall Film Case 220 Mid
Wall Film Case 220 High

Public
DISCUSSION

- Most of the injected AdBlue vaporizes in the gas phase
- Wall film formation declines with increasing temperature
- Simulation of 10 pulse gives a trend, full steady-state is not reached
- Results for 1D
  - Deposition split ratio
  - Film thickness

<table>
<thead>
<tr>
<th>Case</th>
<th>Film mass [%]</th>
<th>Evaporated Spray [%]</th>
<th>Case</th>
<th>Film mass [%]</th>
<th>Evaporated Spray [%]</th>
<th>Case</th>
<th>Film mass [%]</th>
<th>Evaporated Spray [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>220 Low</td>
<td>0.16</td>
<td>46.45</td>
<td>280 Low</td>
<td>0.06</td>
<td>63.25</td>
<td>360 Low</td>
<td>0.15</td>
<td>77.07</td>
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<tr>
<td>220 Mid</td>
<td>3.17</td>
<td>26.89</td>
<td>280 Mid</td>
<td>0.08</td>
<td>63.20</td>
<td>360 Mid</td>
<td>0.24</td>
<td>77.54</td>
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<tr>
<td>220 High</td>
<td>8.53</td>
<td>22.35</td>
<td>280 High</td>
<td>2.97</td>
<td>53.72</td>
<td>360 High</td>
<td>0.34</td>
<td>76.08</td>
</tr>
</tbody>
</table>
Outlook
Transient Driving Cycle Simulation 3D → 1D

Input parameters derived from 3D CFD: split factor, average film thickness (~1/A_{film})

Parameter study: Average film thickness

Wurzenberger, J.C., Nahtigal, A., Mitterfellner, T.: "1D/3D Simulation of Urea Dosing – Deposit Formation and NOx Reduction in Real Driving", SIA POWERTRAIN / ROUEN 2018
SCR Depositions
Conclusion, Outlook

• Chemical Model available to describe Urea decomposition in technically relevant temperature range
• Simulation methodology available to generate meaningful results in reasonable times
• Derivation of deposition rate [g/h] possible
• Deposition margin using divide & conquer method

Ultimate goal of 3D CFD: Generate deposition map for EAS geometry + AdBlue injector to adjust engine calibration (raw emissions)

Use 3D CFD results to calibrate 1D models
• Generate cycle-resolved results in realtime
Thank You

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