Low-dimensional models for after-treatment devices

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Cambridge Particle Meeting, 10 June 2016
Motivation

- Multi-component and multi-level system
- Simulation-based engineering is key

This work focuses on after-treatment model
Flow through monolith

- Surface chemistry
- Interaction with channel walls

Figure from Fogler & Gurmen, Prentice Hall (2010)
Wall flow monolith

- Particle filtration
- Soot-catalyst interaction

Figure from M.V. Twigg, Catalysis Today 163 (2011) 33-41
Ideal reactor network

Gas phase reactions

Heterogeneous reactions

Surface phase reactions
Ideal reactor network

Heat of reaction

Gas-surface heat transfer

Surface-ambient heat transfer
Ideal reactor network

- Arbitrary connections
  - Flexibility
- Extensible
  - Additive control
  - Higher dimension possible
Ideal reactor network

- Reaction mechanisms from literature
  - Single universal mechanism
    - Elementary reactions
    - Global reactions
• Main reactions
  - $2\text{CO} + \text{O}_2 \rightarrow 2\text{CO}_2$
  - $2\text{C}_3\text{H}_6 + 9\text{O}_2 \rightarrow 6\text{CO}_2 + 6\text{H}_2\text{O}$
  - $2\text{NO} + \text{O}_2 \leftrightarrow 2\text{NO}_2$
Diesel Oxidation Catalyst

- Mechanism
  - Koop & Deutschmann (2009)
  - Pt/Al$_2$O$_3$
  - 73 elementary reactions

Mechanism from Koop & Deutschmann, Applied Catalysis B: Environmental Vol. 91 (2009), 47-58.

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DOC verification

Experimental data from Koop & Deutschmann, Applied Catalysis B: Environmental Vol. 91 (2009), 47-58.

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• Cake formation
  - $C \rightarrow C^*$

• Regeneration
  - Active: $5C^* + 4O_2 \rightarrow 2CO + 3CO_2$
  - Passive: $5C^* + 9NO_2 \rightarrow 9NO + CO + 4CO_2$
Diesel Particulate Filter

- Regeneration reactions
  - 2 Global reactions
- Particulates
  - Elementary carbon; ash possible

Active regeneration

Particulate Filter

Temperature (K)

Deposited mass (g)

Time (s)

Inlet gas temperature
Wall temperature
Deposit mass

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Selective Catalytic Reduction

- Main reactions
  - $4\text{NO} + 4\text{NH}_3 + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$  
  (Standard SCR)
  - $\text{NO} + \text{NO}_2 + 2\text{NH}_3 \rightarrow 2\text{N}_2 + 3\text{H}_2\text{O}$  
  (Fast SCR)
  - $6\text{NO}_2 + 8\text{NH}_3 \rightarrow 7\text{N}_2 + 12\text{H}_2\text{O}$  
  (NO$_2$ SCR)
Selective Catalytic Reduction

- Side reactions
  - $2\text{NO} + \text{O}_2 \leftrightarrow 2\text{NO}_2$
  - $2\text{NO}_2 + 2\text{NH}_3 \rightarrow \text{N}_2 + \text{N}_2\text{O} + 3\text{H}_2\text{O}$
Selective Catalytic Reduction

- Mechanism
  - Olsson et al. (2008)
  - Cu-ZSM-5
  - 8 global reactions
SCR verification


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SCR verification

Inlet NO$_2$% 0% 20% 40% 50% 60% 80% 100%

Outlet concentration (ppm)

- **Experimental, NO$_2$**
- **This work, NO$_2$**
- **Experimental, N$_2$O**
- **This work, N$_2$O**

500ppm NH$_3$
500ppm NOx
350°C


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Flux of reaction

- NO Oxidation
- Standard SCR
- Fast SCR
- NO₂ SCR
- N₂O Formation

Inlet NO₂ content:

- 0%
- 20%
- 40%
- 60%
- 80%
- 100%

Flux of reaction (mol/m³ s)
Parameter scan

**deNOx efficiency**

500ppm NOx
50% NO₂
350 °C

**NH₃ slip**

**N₂O slip**
Multi-devices

- Boundary conditions
  - 7L Diesel engine
  - SRM Engine Suite
  - Smallbone et al. (2013)
  - 4 operating points

Oxidation Catalyst → Particulate Filter → Reduction Catalyst

Reductant

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Operating points

Base case

Cold

High speed

High torque

Normalized concentration

Oxidation Catalyst → Particulate Filter → Reduction Catalyst

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Summary

• Can do chemically driven systems
• Fast → Allow global analysis
• Improve consideration of
  ▪ Heat transfer
  ▪ Particle information
• More complicated device
  ▪ Catalysed particulate filter
Acknowledgements