

Technical University of Denmark



## Modeling the Automotive SCR Catalyst

Åberg, Andreas; Widd, Anders; Abildskov, Jens; Huusom, Jakob Kjøbsted

*Publication date:*  
2015

*Document Version*  
Peer reviewed version

[Link back to DTU Orbit](#)

*Citation (APA):*  
Åberg, A., Widd, A., Abildskov, J., & Huusom, J. K. (2015). Modeling the Automotive SCR Catalyst. Poster session presented at 19th Nordic Process Control Workshop, Trondheim, Norway.

## DTU Library

Technical Information Center of Denmark

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Modeling the Automotive SCR Catalyst

Andreas Åberg\*, Anders Widd\*\*, Jens Abildskov\*, Jakob Kjøbsted Huusom\*

\*Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

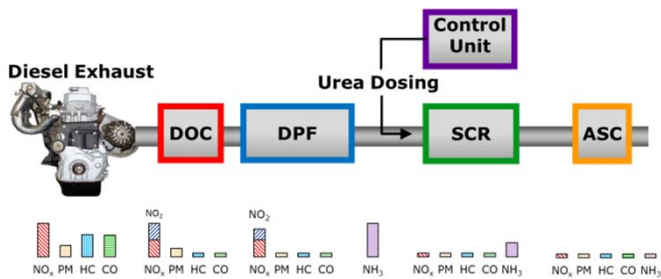
\*\*Haldor Topsøe A/S, Nymøllevvej 55, DK-2800 Lyngby, Denmark



## 1. Introduction

Heavy duty diesel vehicles handle a substantial part of the world's transportation. Harmful pollutants are formed, such as nitrogen oxides, hydrocarbons, particulate matter, and carbon monoxide. It is of great importance to reduce emissions due to urban air quality, and new legislation.

The unit of interest for this project is the SCR catalyst. NOx is removed through Selective Catalytic Reduction (SCR) using NH3 as a reducing agent. Challenges with this technology include dosing the right amount of urea to reach sufficient NOx conversion, while at the same time keeping NH3-slip from the exhaust system below the legislation. This requires efficient control algorithms. Model based methods are an attractive method because they are modular, flexible with regards system configurations, etc.



## 2. Model

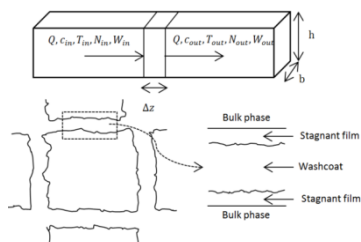
The equations describing the SCR catalyst can be divided into bulk equations that describes the flow through the main channels, and washcoat equations that describe the washcoat phase. Model parameters have been estimated with correlations. The reaction kinetics were described by Arrhenius expressions, with parameters that were calibrated using experimental data.

$$\frac{\partial c_{b,i}}{\partial t} = -u \frac{\partial c_{b,i}}{\partial z} - \frac{4k_g}{b} (c_{b,i} - c_{wc,i})$$

$$\frac{\partial c_{wc,i}}{\partial t} = \frac{4k_g}{b} (c_{b,i} - c_{wc,i}) + \sum_i r_i$$

$$\frac{\partial T_b}{\partial t} = -u \frac{\partial T_b}{\partial z} - \frac{4h_{heat}}{b\rho_b c_{p,b}} (T_b - T_{wc})$$

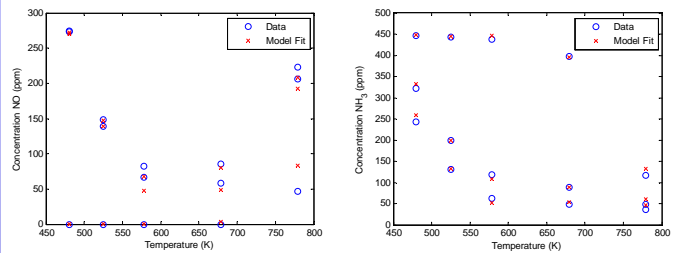
$$\frac{\partial T_{wc}}{\partial t} = \frac{4h_{heat}}{b\rho_{wc} c_{p,wc}} (T_b - T_{wc}) + \sum_i \Delta H_{r,i} r_i$$



## 4. Results

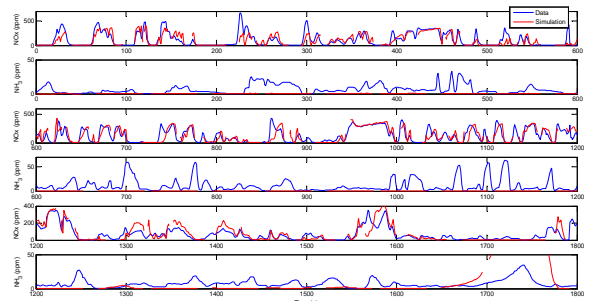
### Calibration

Calibration of kinetic parameters was done with isothermal steady state benchscale monolith data. Residuals can be seen in the two figures below. The residuals are small for both NO<sub>x</sub> and NH<sub>3</sub>, suggesting a good fit. The cross-correlation was generally low.



### Validation

Validation of the calibration was done by simulating a full cycle from the European Transient Cycle (ETC) with a full-scale monolith, and comparing to experimental data. NO<sub>x</sub> simulation follows data well over a large range of operating conditions, but the NH<sub>3</sub> simulation needs improvement.



## 5. Conclusions

A first principle model has been derived. The model was calibrated with steady-state small-scale monolith data at isothermal conditions. The full-scale transient validation showed that the model was able to accurately predict the monolith output of NO<sub>x</sub>. The NH<sub>3</sub>-slip prediction was however not satisfactory.

### References:

- M. Koebel, M. Elsener, M. Kleeman, Urea-SCR: a promising technique to reduce NO<sub>x</sub> emissions from automotive diesel engines, Catal. Today 59 (2000) 335-345.
- Pär L.T. Gabrielsson, Urea-SCR in automotive applications, Top. Catal. 28 (2004) 1-4.