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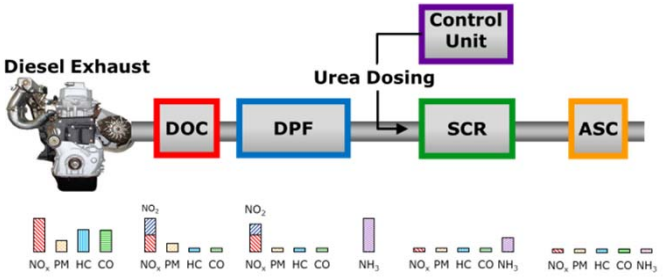
1. Introduction

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

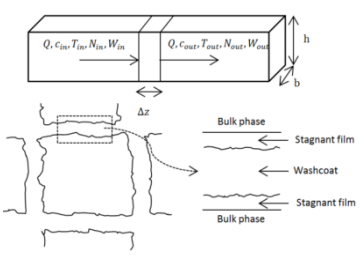
The equations describing the SCR catalyst can be divided into bulk equations that describes the flow through the main channels, and washcoat equations that the describe washcoat phase. Model parameters has been estimated with correlations. The reaction kinetics were described by Arrhenius expressions,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

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

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

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

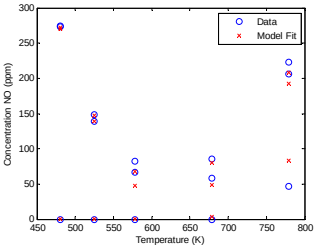
$$\frac{\partial T_{wc}}{\partial t} = \frac{4h_{heat}}{b\rho_{wc} c_{p,wc}}\left(T_b - T_{wc}\right) + \sum_i \Delta H_{r,i} r_i$$

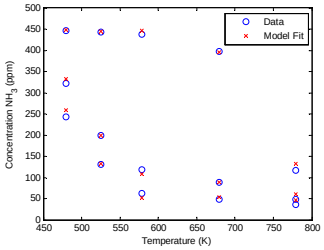


4. Results

Calibration

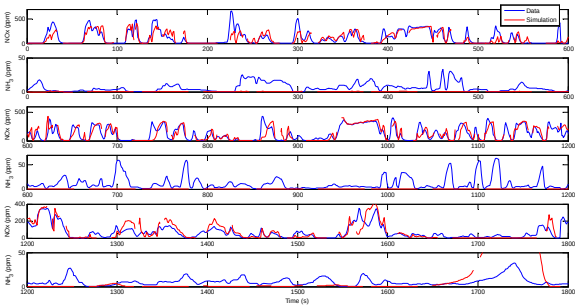
Calibration of kinetic parameters was done with isothermal steady state benchscale monolith data. Residuals can be seen in the two figures below. The residuals are small for both NOx and NH3, suggesting a good fit. The cross-correlation was generally low.





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. NOx simulation follows data well over a large range of operating conditions, but the NH3 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 NOx. The NH3-slip prediction was however not satisfactory.

References:
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Pär L.T. Gabrielsson, Urea-SCR in automotive applications, Top. Catal. 28 (2004) 1-4.