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A Reduced Order Model of NH_3-SCR Monolithic Converters for Mobile Applications

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Highlights

- A reduced order model for real-time simulation of NH_3-SCR converters is derived.
- Reduced model achieve accuracy comparable to a state-of-the-art chemical-physical model
- Reduced model is up to 2 orders of magnitude faster with respect to the reference model
- Reduced model is suitable for real-time model based control of SCR converters

1. Introduction

NH_3-SCR currently represents the leading technology for NOx abatement from lean burn and Diesel engines. NOx emission limits from mobile sources have become more stringent with the current legislations. Consequently, accurate model predictions and on-board controls of the engine after-treatment systems are required to comply with the NOx emissions limits. In this work, Control Oriented Models (COM) for Selective Catalytic Reduction (SCR) have been studied as a strategy to provide accurate simulations with low computational costs which are suitable for fast model calibration and for on-board control purposes. In this work, a new type of COM is developed. To reduce the computational costs, a combination of explicit and implicit Euler methods has been implemented, using a simplified approach to calculate the region of stability of the explicit method. Moreover, a detailed comparison in terms of accuracy and computational costs between a reference complete SCR monolith converter model and the reduced COM will be performed for different engine tests cycles, comprising cold start transients for both light and heavy-duty diesel engines. In these tests, a significant decrease in the computational time for COM is demonstrated with respect to the reference full model, with comparable accuracy.

2. Methods

To check the accuracy of COM predictions, a state-of-the-art, already extensively validated chemical-physical model of SCR monolithic converters [1] has been used as a reference. The adopted reference model was developed to simulate washcoated Fe- and Cu-zeolite catalysts as well as extruded V-based catalysts. Accordingly, it accounts for both external gas-solid mass transfer and intraporous diffusion within the catalytic phase, based on a fully transient two-phase 1D+1D mathematical description of SCR honeycomb monolith reactors, specifically adapted for mobile SCR applications.

3. Results and discussion

A reduced 1D+1D heterogeneous PFR model of the SCR monolithic converter, embedded with a fully detailed kinetic scheme comprising material balances for gaseous (NH_3, NO, NO_2 and H_2O) and adsorbed (NH_3*, NH_4NO, and H_2O*) species has been developed. This allows to account for the most important typical features of the SCR reactivity, such as e.g. ammonium nitrate deposition and decomposition. Both internal and external mass transport phenomena, that may become important depending on the operative conditions, are included, while maintaining the explicit nature of the formulation. Finally, to correctly describe the heat up dynamics of the converter, a suitable energy balance is also included. The resulting model has been derived under some necessary simplifying assumptions: i) mass and energy storage in the gas phase are negligible; ii) axial mass and thermal diffusion within the gas phase are negligible; iii) the wall temperature is uniform within each discretization element but varies along the reactor length; iv) heat conduction in longitudinal direction along monolith walls is negligible.

As a first interesting theoretical result, we demonstrate that the utilization of the orthogonal collocations method [2] with a single interior point for the numerical solution of the internal transport field in the washcoat is formally equivalent to the approach of internal mass transfer coefficients presented by Balakotaiah [3]. This directly follows from the coefficients used for the approximation of the derivatives.

Concerning numerical results, Figure 1 compares the simulated outlet concentration profiles of the reduced and reference models for the simulation of a typical engine cycle, a cold start WHTC. The cycle is representative of low temperature conditions during a heat up transient. Clearly, the reduced model nicely reproduces the reference model results. What is worth emphasizing is the difference in computational performances between the two models: the reference model completes the whole simulation (1800 s) in about 480 s, with a time ratio of 0.268; the reduced model takes only 3 s to complete the cycle, with a time ratio of $1.7 \cdot 10^{-3}$. The speed up factor is therefore in the order of 160 times. Interestingly the overall deviation between the two models, evaluated as the Root Mean Squared Error (RMSE) over the whole simulation time, is less than 10 ppm for each concentration profile.

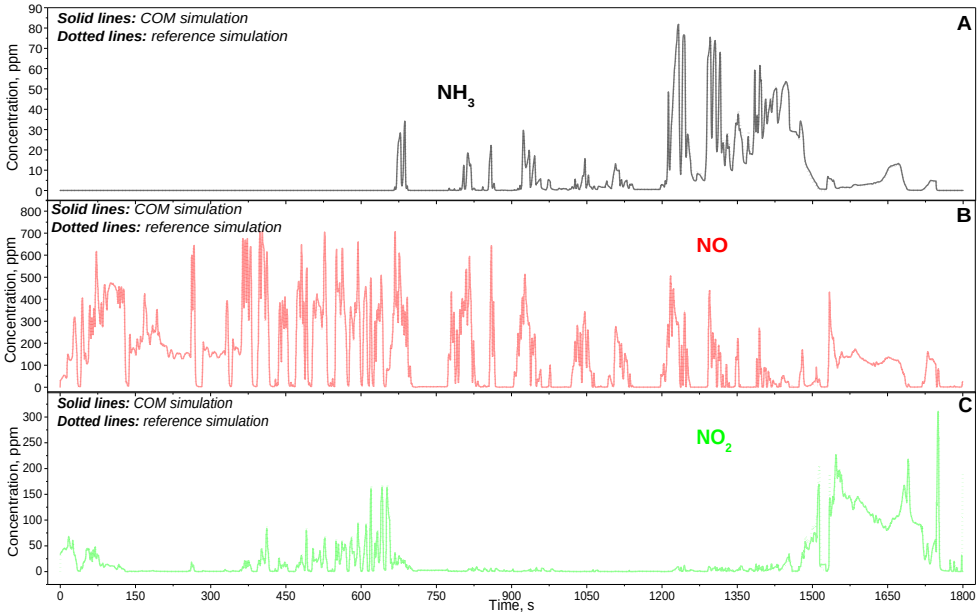

Figure 1. WHTC with cold startup simulation. Outlet concentration profiles: A) NH_3; B) NO; C) NO_2.

4. Conclusions

We have derived a reduced model suitable for real-time simulation of SCR catalytic converters in Urea/NH_3-SCR aftertreatment systems. The reduced model satisfies all the requested objectives, such as: i) explicit and stable mathematical formulation; ii) inclusion of a fully detailed kinetic scheme able to account for the most important features of SCR reactivity; iii) description of both internal and external mass transport phenomena, which become important at high temperatures; iv) inclusion of an energy balance to correctly describe the heat up dynamics of the converter. It has been successfully validated by comparison with a reference full model, demonstrating a significant reduction of the computational time (from 1 to 2 orders of magnitude, depending on the conditions) while retaining a satisfactory accuracy.

References

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Keywords
NH_3-SCR; monolithic converters; control oriented model; real time simulation; aftertreatment simulation.