Mathematical modelling of combined DOC, NSRC and (C)DPF system for diesel exhaust aftertreatment

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Introduction
Subjects of the work are mathematical modelling and simulation study of the combined system of catalytic converters, used for the after- treatment of exhaust gases from diesel engines. The studied system consists of NOx storage and reduction catalyst (NSRC) - operated in a periodic lean/rich regime, diesel oxidation catalyst (DOC) and non-catalytic particulate filter (C-DPF). This system is used for the abatement of NOx, CO, hydrocarbons and diesel particulate matter in exhaust gases from engines burning fuel mixture with excess of air, i.e. compression-ignition type (Diesel) engines.

Mathematical models
Detailed mathematical models of the wall-flow (C-DPF) and the flow-through (DOC & NSRC) can be used individually or could be integrated for simulations of the interconnected aftertreatment system or, e.g., CTP®.

Wall-flow model - Diesel particulate filter (C-DPF)
The filter model is derived from the original equations proposed by Bissett. The model considers the following partial differential equations:

\[
\frac{\partial}{\partial t} \varphi \left( x, y, z, t \right) + \frac{\partial}{\partial x} \left( J_1 \varphi \right) + \frac{\partial}{\partial y} \left( J_2 \varphi \right) + \frac{\partial}{\partial z} \left( J_3 \varphi \right) = \frac{\partial}{\partial x} \left( \lambda \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \lambda \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \lambda \frac{\partial \varphi}{\partial z} \right) + F
\]

where \( \varphi \) is the concentration of the substance, \( J \) is the flux, \( \lambda \) is the diffusivity, and \( F \) is the source term.

Numerical solution
Numerical solution of partial differential equations of the DPF model is based on the discretization of the set of partial differential equations. In the case of the DOC model, the reaction rates of NOx, CO, hydrocarbons and diesel particulate matter are included using the finite differences method, with equi-mass changes in chosen finite volumes.

References