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Simulation of a Three-Way Catalyst Using a Transient Multi-Channel Model

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Introduction

The three-way catalyst (TWC) is the most common catalyst for gasoline engine exhaust gas after treatment and its conversion effects have been simulated in previous works using single-channel approaches [1] and detailed kinetic models [2]. In addition to the these concepts multiple representative catalyst channels with and without radial inlet temperature variations are presented here.

Setup

Emissions and temperature measurements of a Pd/Rh coated TWC are performed. The inlet emissions are measured at a common four-stroke engine and then fed into the catalytic converter.

For the modeling of the catalyst 9 channels are used where each channel is split into 10 equidistant cells as shown in Figure 2. Three different simulations are performed with detailed chemistry and varying transient inlet temperatures shown in Figure 1.

In the first case a radial uniform inlet temperature is fed into the catalyst. In the second case, it is assumed that the inlet flow center (channel 5 in Figure 2) is hotter than the surrounding 8 channels. In the third case the highest temperature inlet stream is assigned to channel 2.

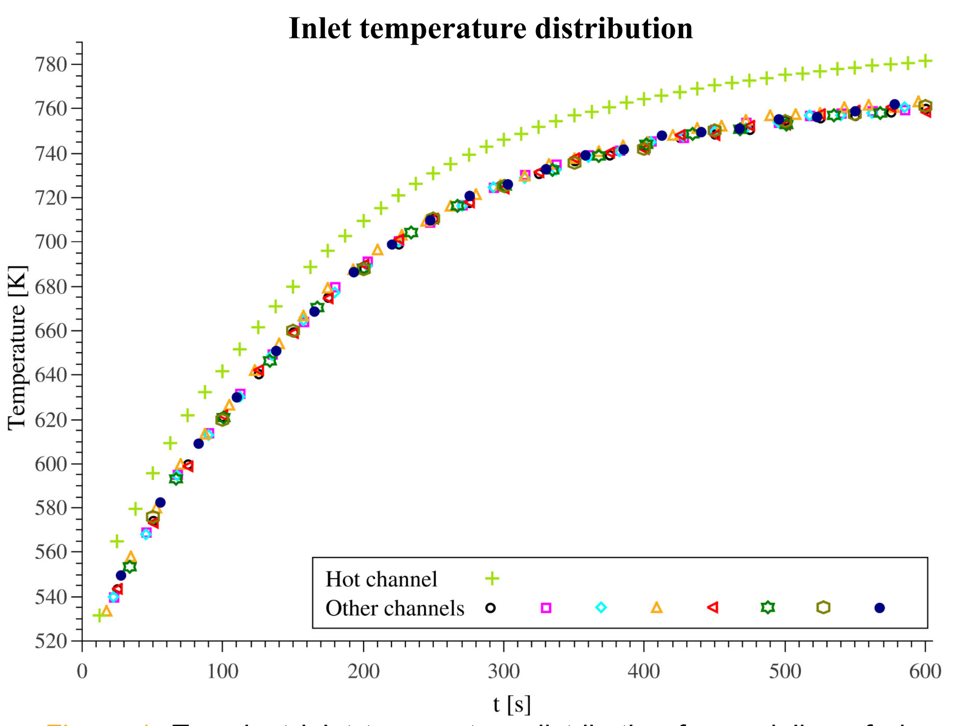

Figure 1: Transient inlet temperature distribution for modeling of nine channels with the multi-channel approach.

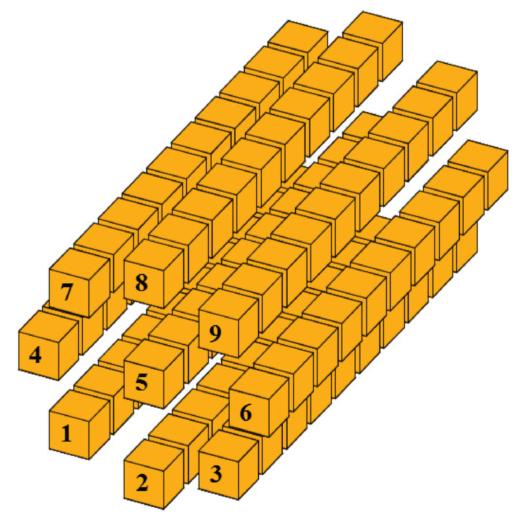

Figure 2: Representative channel positions for the multi-channel setup.

Modeling approach

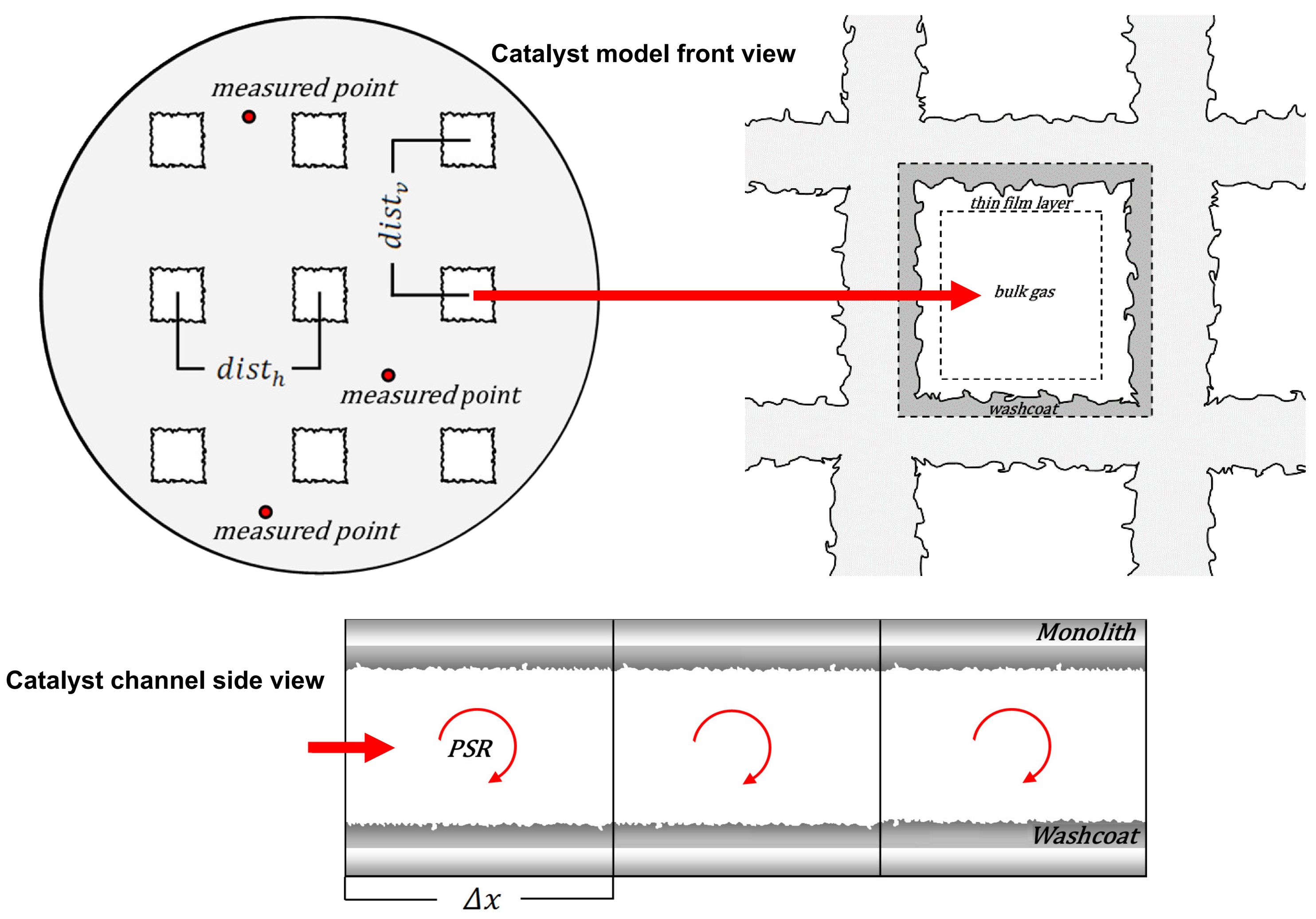

Figure 3: Schematic illustration of the modeling approach [3]

The simulations are carried out with LOGEsoft LS1.08.

Modeling results

The light-off temperature of the catalyst is determined between seconds 80 and 90. Second 85 is chosen as representative time for all three emissions. In Figures 4-7 the modeling results at representative light-off are shown along the catalyst cross-section.

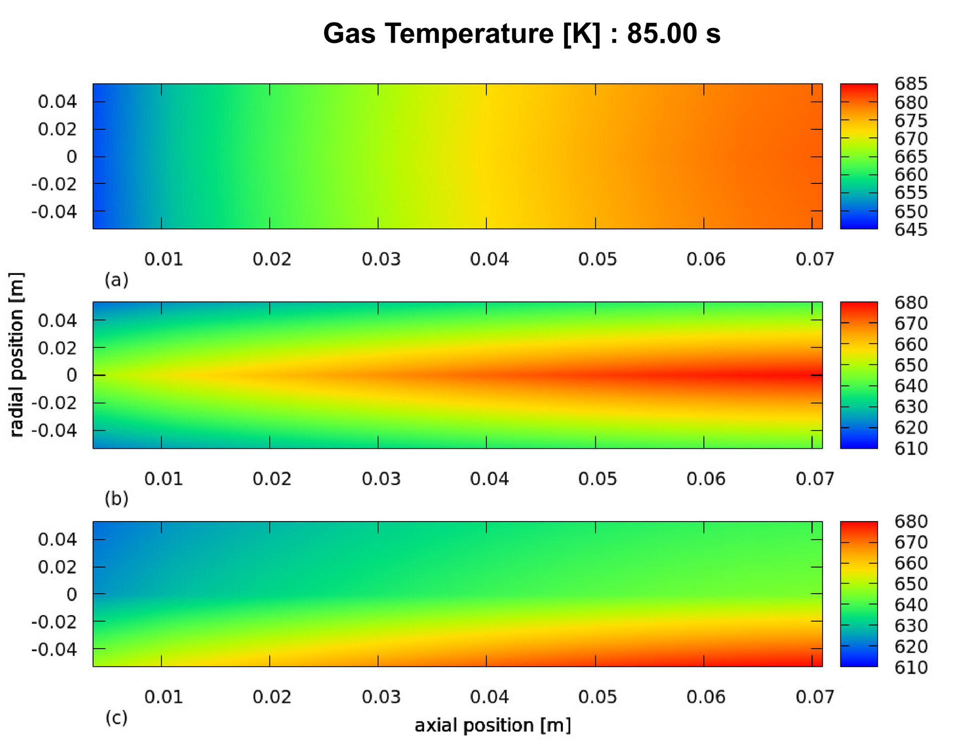

Figure 4: Bulk gas temperature at representative catalyst light-off for (a) uniform temperature, (b) temperature distribution with a hotter flow core and (c) distribution with a hotter second channel.

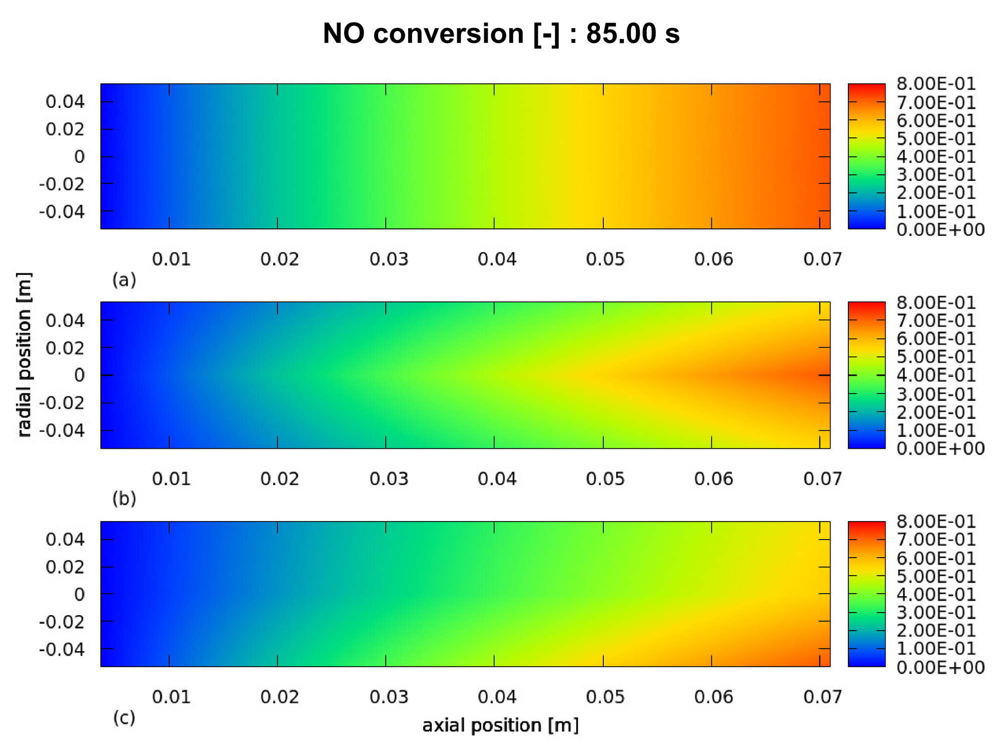

Figure 5: NO conversion at catalyst light-off for (a) uniform temperature, (b) temperature distribution with a hotter flow core and (c) distribution with a hotter second channel.

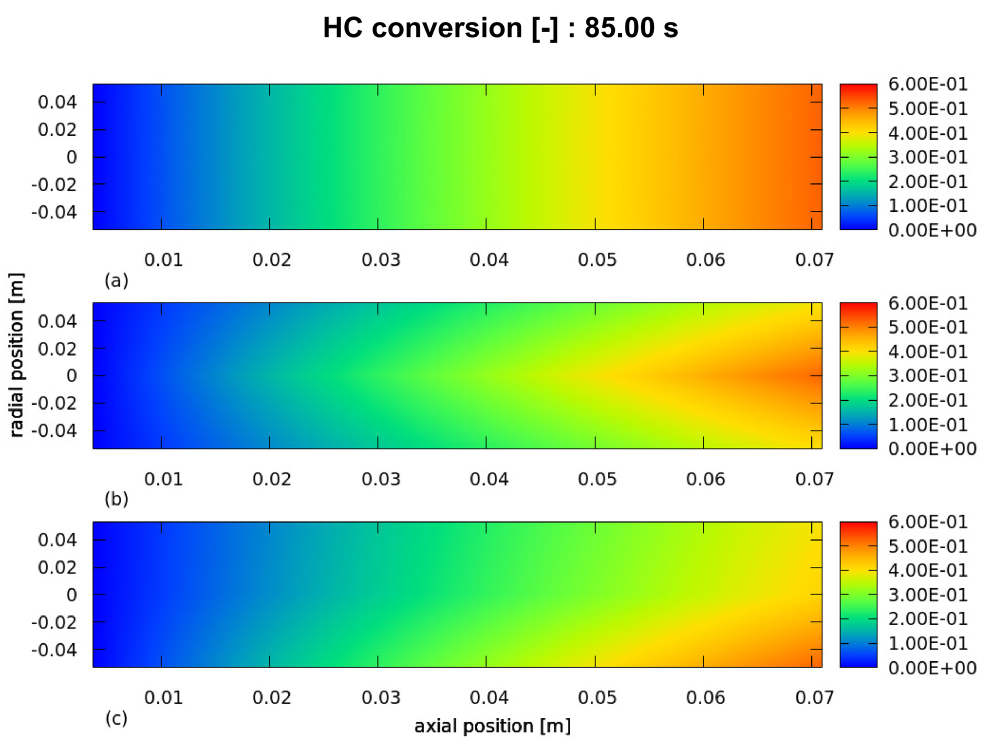

Figure 6: HC conversion at catalyst light-off for (a) uniform temperature, (b) temperature distribution with a hotter flow core and (c) distribution with a hotter second channel.

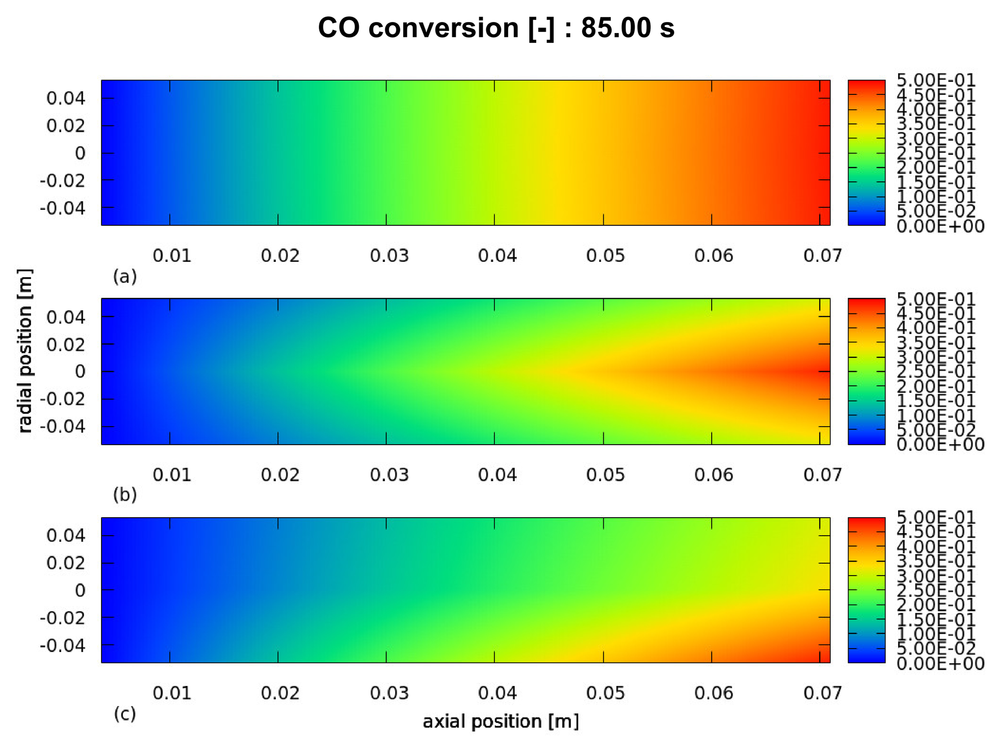

Figure 7: CO conversion at catalyst light-off for (a) uniform temperature, (b) temperature distribution with a hotter flow core and (c) distribution with a hotter second channel.

In Figure 8 it is visible that the simulation results with temperature distribution better agree with the experimental outlet temperature data from second 100 on than the simulations with uniform inlet temperature. This can be explained by the more physical approach of radial temperature variations in the inlet flow. Due to the improved temperature model, the simulation results of after catalyst emissions when using the two different temperature distribution models as shown in Figure 9 also better fit the experimental data. The differences between the different temperature distribution profiles are negligible.

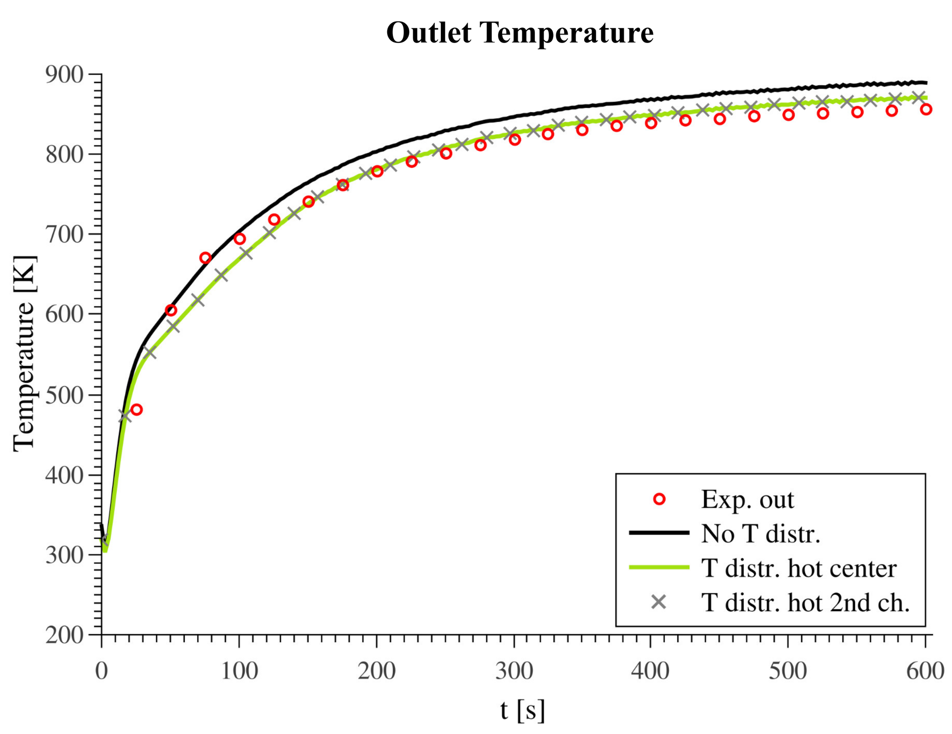

Figure 8: Transient outlet temperature comparison with and without radial temperature distribution.

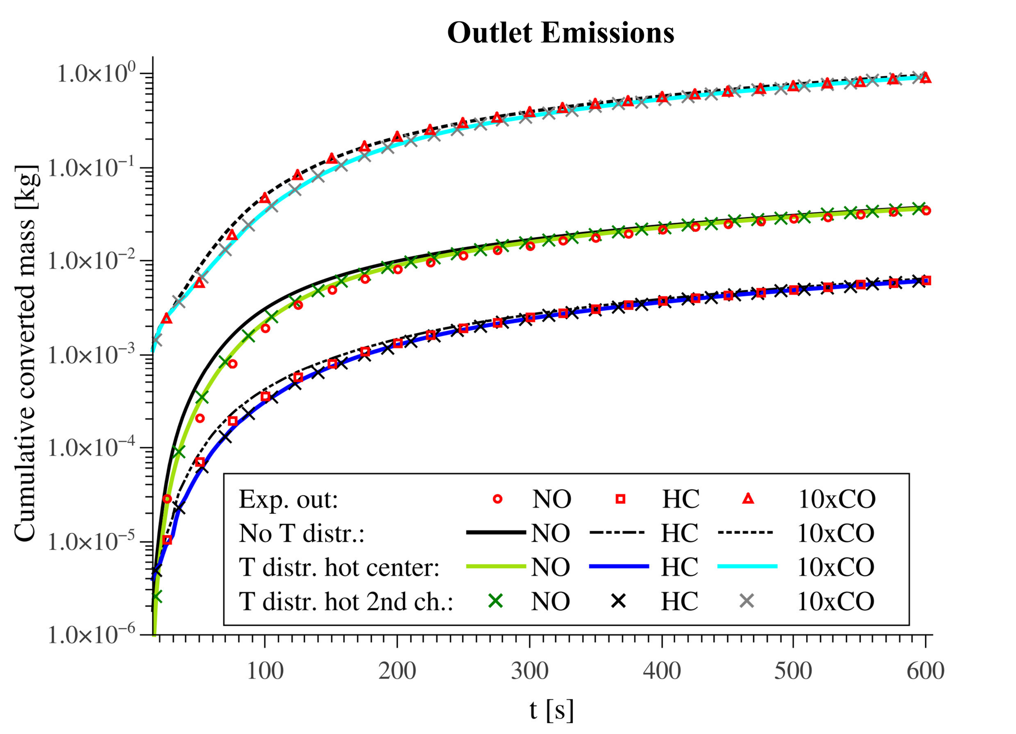

Figure 9: Transient cumulative converted mass emissions of hydrocarbons, carbon monoxide and nitrogen oxide for modeling of nine channels with the multi-channel approach.

Conclusions

The presented multi-channel model shows a good agreement with the experimental data. Taking radial heat transfer into account is useful to improve the performance of the model for most of the predicted emissions and the predicted outlet temperature. It offers an alternative, more physically realistic concept for modeling of heterogeneous catalytic converters with low computational cost.

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[3] J. Aslanjan, C. Klauer, C. Perlman, V. Günther, F. Mauss, Simulation of a three-way catalyst using transient single and multi-channel models, SAE Technical Paper, (2017), 2017-01-0966.

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