Spatio-temporal dynamics of oxygen storage and release in a three-way catalytic converter with axially non-uniform catalyst activity

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Abstract

Three-way catalytic converters (TWC) are exhaust after-treatment systems commonly used in stoichiometry operated gasoline vehicles. Within a narrow zone around stoichiometry, the TWC can simultaneously oxidize CO and HC while reducing NOx. In order to buffer slight excursions from stoichiometric operation and abate emission breakthrough, oxygen-storing components, such as ceria, are added in TWC to store oxygen in the fuel lean phase and release it in the fuel rich phase.

Axially non-uniform catalyst activity of a TWC may result from non-uniform platinum-group metal (PGM) and/or ceria loading or non-uniform deactivation. For fixed amounts of total PGG and ceria loading, proper redistribution (with more catalyst near the inlet) favors fast light-off of the TWC and reduces cumulative cold-start emissions substantially [1]. Local temperature peaks due to certain operations (e.g. cold start, sudden acceleration, etc.) may cause non-uniform aging of the catalyst which leads to different TWC cold start dynamics from a uniformly aged one.

In this work, we use a recently developed physics based reduced-order one-dimensional transient model to study the spatio-temporal dynamics of oxygen storage and release in a TWC with axially non-uniform catalyst activity. For a uniform catalyst activity case, the TWC model is validated using emission data collected in a vehicle over multiple drive cycles. The internal mass transfer approximation is confirmed by comparing with a detailed washcoat diffusion-reaction model and is observed to be consistent for all practical purposes. Simulations are conducted for multiple cases such as cold start and fast lean-rich cycling to study oxygen storage dynamics, transient temperature profile and emission breakthrough in the TWC. Cold start and fast cycling simulation results for the uniform catalyst activity case are shown in Fig. 1-2. The results for non-uniform catalyst activity case are compared with the uniform case.

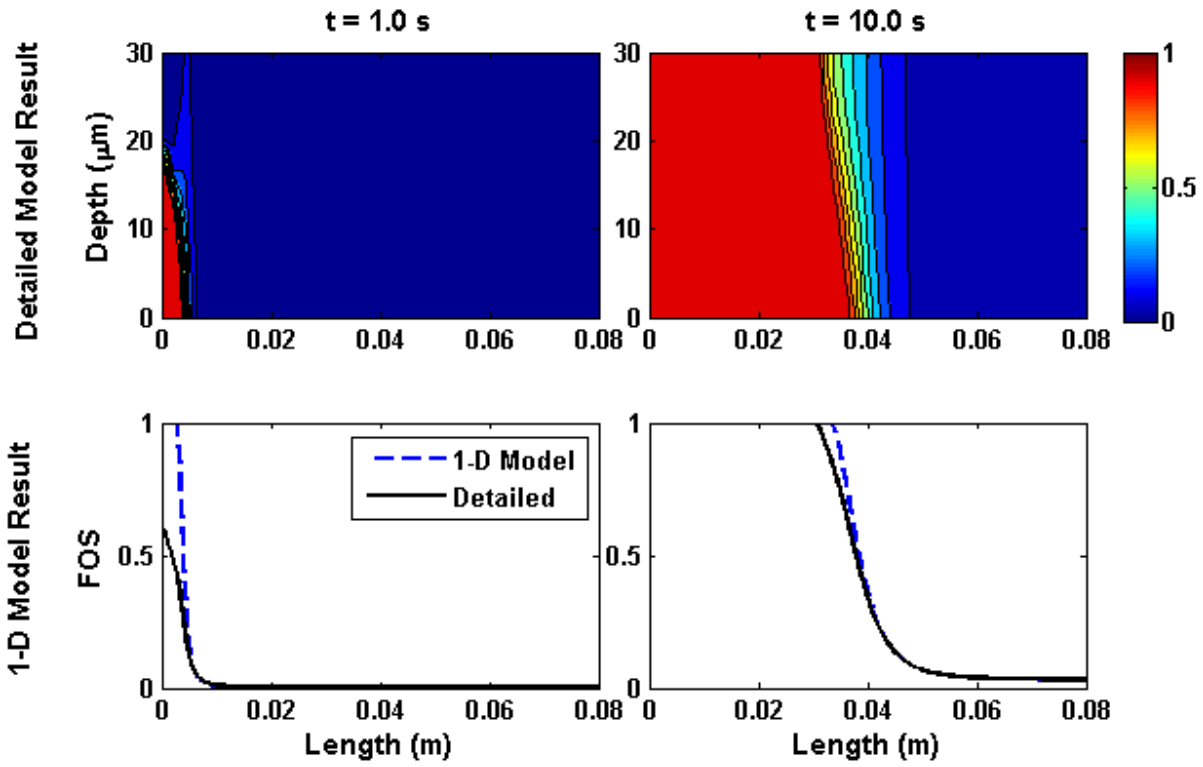


Fig.1 Profiles of fractional oxidation state (FOS) under cold start condition.

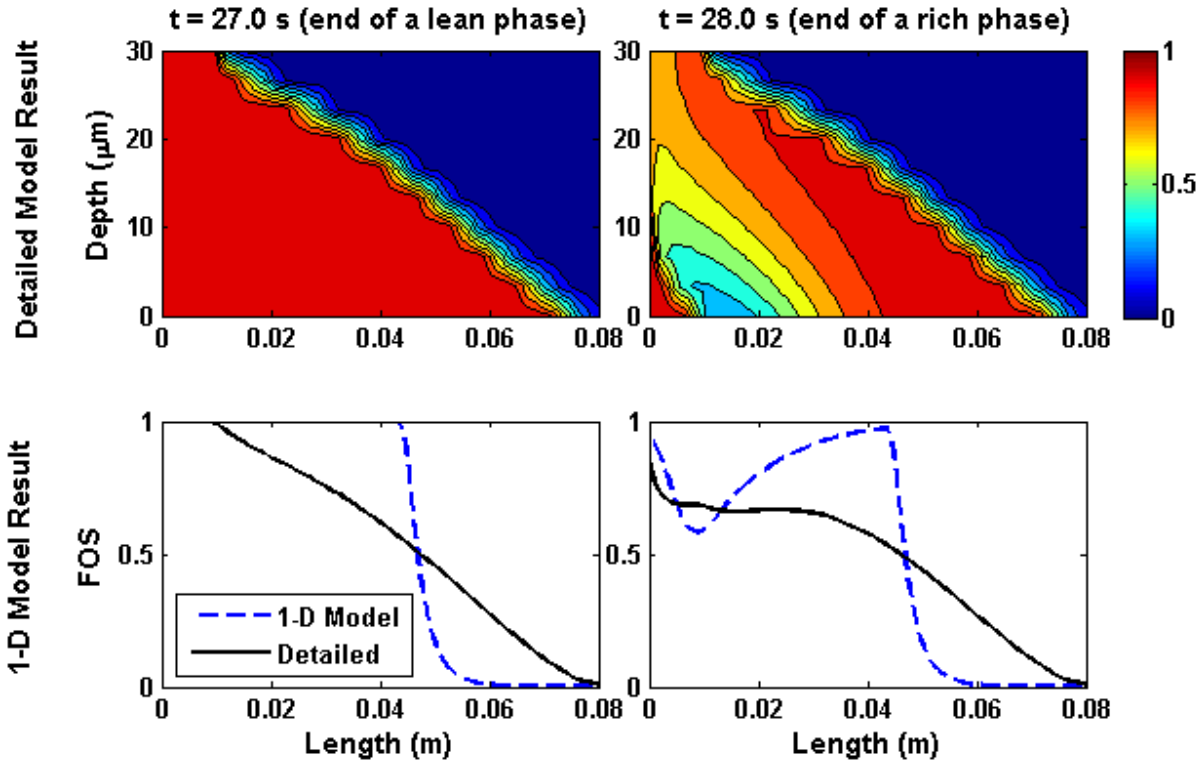


Fig.2 Profiles of FOS during fast lean-rich cycling.

Reference

1. Ramanathan, K., West, D. H., & Balakotaiah, V. (2004). Optimal design of catalytic converters for minimizing cold-start emissions. Catalysis today, 98(3), 357-373.