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Oscillations and Hysteresis during Hydrocarbon Oxidation on a Diesel Oxidation Catalyst: Predictive Model

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Abstract

Dodecane oxidation on zeolite beta (BEA) was studied on a diesel oxidation catalyst (DOC) comprising Pt-Pd/Al_2O_3. Oscillatory CO_2 formation under steady-state and transient conditions was studied by spatially-resolved mass spectrometry (SpaciMS) and coherent optical frequency domain reflectometry (c-OFDR) [1]. The CO_2 oscillations were accompanied by local temperature fluctuations during the steady state and temperature-programmed oxidation. The coupling between hydrocarbon sorption and oxidation, the proposed underlying mechanism for the oscillatory behavior, is investigated using a monolith reactor model. Using independently measured dodecane oxidation and sorption kinetics, the model predicts most of the experimental features, including the existence and amplitude of the oscillations. The model also correctly predicts the existence of an observed hysteresis during temperature ramp-up/ramp-down experiments. A non-dimensional map provides a predictive guide for the existence of oscillations. In addition to providing understanding and prediction of the spatiotemporal phenomena, the model analysis suggests a way to decrease the hydrocarbon slip (emissions) during temperature ramp-down.

Keywords: Beta zeolite; Oxidation; Hydrocarbon Trap; Oscillation; Diesel