

Math-Based Approach to the Design and Optimization of Vehicle Emission Control Systems

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In the face of the ever-tightening exhaust emission standards over the next decade or so and the rapidly rising noble metal prices, it is of critical importance to further improve the performance and durability of a catalytic converter while reducing both its noble metal content and development time. An effective way to meet these challenges is to use math-based tools for the development of emission control systems with optimum cost/performance.

In this presentation, we first briefly discuss the 1-D “single-channel” monolith converter model and the more comprehensive three-dimensional model, with particular emphasis on the comparison of the features included and their capabilities/limitations. Although the 3-D model would be required for the analysis of thermal stress and fatigue in the monolith converter assembly, the simpler 1-D model has been shown to be adequate in describing the transient conversion performance of a monolith converter. The 1-D “single-channel” model with global rate expressions has been used extensively at General Motors to address a variety of emission control system design, optimization and implementation issues, and some examples of the model applications will be discussed.

Although the monolith model with global kinetics provides a useful design tool, we need converter models with more detailed kinetics based on elementary reaction steps in order to describe the reaction events and fast transients more accurately. In these models, reaction kinetics is accounted for by including elementary reactions occurring on the catalyst surface (such as adsorption, desorption and surface reaction), rather than by global rate expressions. Such an elementary reaction step-based approach is better suited to handling a situation where rate-determining steps are likely to change within the converter (e.g., as a result of very high conversions and/or temperature change), allows one to easily extend/adapt the model to more complex reaction systems and/or catalyst formulations, and can be extrapolated with more confidence to outside the ranges where experimental data exists. However, such a fundamental model requires *quantitative* understanding of the reaction mechanism, including the rate constants for all the elementary reaction steps involved. The elementary reaction step-based modeling approach will be illustrated for simple reaction systems relevant to automobile exhaust catalysis, and challenges and future research needs associated with its application to the actual exhaust environment will be discussed.