

## First-principle Modeling of a Three-Way Catalytic Converter System

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Three-way Catalytic converter (TWC) system has been widely used and it can meet the gradually stricter regulations against automobile exhaust emissions. This after-treatment system eliminates carbon monoxide, hydrocarbon and nitrogen oxides from gasoline engine's exhaust emission gas. A high-fidelity model of catalytic converter system model can reduce the cost of developing catalysts in the industry. In this study, we propose an one-dimensional model for TWC system. The proposed first-principle model considers 34 reactions including oxidative reactions over platinum group metal and oxygen storage. A dual-site OSC model is also considered in order to demonstrate two oxygen storage site (surface ceria and sub-surface ceria). Particle swarm optimization is used to estimate kinetic parameters using experimental data including rich condition and lean condition. The suggested one-dimensional model is validated by actual driving data.