June 13, 2022

N.E. CHEMCAT Awarded FY2022 CMAJ Technology Award for the "Modeling on a Three-Way Catalyst Used in Series Hybrid Electric Vehicles (SHEVs)"

Successfully constructed a model on "TWC catalyst purification reactions" against changes in catalyst activation caused by exhaust gas temperature and atmospheric fluctuations at "cold start" and "restart" conventionally difficult to predict

N.E. CHEMCAT CORPORATION (Head office: Minato-ku, Tokyo; Representative Director & President Matsuru Kushida) is pleased to announce that it was awarded the **FY2022 CMAJ Technology Award** for the "Modeling on a Three-Way Catalyst used in Series Hybrid Vehicles (SHEVs)." The Award was granted from Catalyst Manufacturers Association, Japan (CMAJ) in the Award Ceremony which was held on-line on June 9, 2022.

With the worldwide strengthening of environmental regulations, the number of processes in designing and developing automobiles is increasing dramatically to accommodate diversified powertrain systems and sophisticated functionalities. More automotive companies are implementing and utilizing Model Based Development (MBD) to streamline the development process, and there is an urgent need to construct models that can provide versatile estimation accuracy. However, because three-way catalysts (TWC), which is one of the most important elements in emission purification systems, provide a highly complicated reaction path, models that can reproduce the entire process from oxidation & reduction to oxygen storage capacity (OSC) reactions and residual products are yet to be established. In particular, models that can reproduce the change in performance from redox of platinum group metals (PGMs) are extremely limited.

As the mobility industry is shifting rapidly towards EV, hybrid electric vehicles (HEVs) will become an increasingly important option. In this study, we focused on the **emission purification system for SHEVs** which we anticipate growth in market shares. SHEV engines can be used exclusively for power generation, so **exhaust gas from SHEV engines is distinctive** because there is a trend of iterated intermittent steady-state engine operation at a specific high-efficiency point and engine stop. By investigating the redox behavior of the catalyst, we successfully reproduced the purification performances under repeated intermittent conditions as well as under versatile operation conditions, and **constructed an innovative three-way catalyst reaction model** that can achieve high prediction accuracy.

In particular, we modelled the behavior in which the catalyst is reduced and activated in a phased manner from the initial oxidized state based on the exhaust gas temperature and air excess ratio. Then, by **introducing a control method to produce changes in the rate constant based on the redox of the catalyst surface due to atmospheric fluctuation**, we were able to **achieve favorable prediction accuracy of emission gas amounts at the catalyst outlet** throughout the transient mode tests.

In view of the strengthening of emissions gas regulations ahead, this model can provide estimations of ammonia (NH_3) and nitrous oxide (N_2O) which are considered to be added to the regulations. Furthermore, through the experiments and calculations used in the model construction process, we gained valuable expertise, including the specific reaction mechanism during the light-off process, which can be utilized in the design of catalysts and development of emission purification systems. The established model was appraised as it could be utilized in the model based development of emission purification systems for HEVs, which led us to win this award.

Going forward, N.E. CHEMCAT will contribute to the accelerating model based development in the designing of automobiles.

■ Outline of the Study (The modeling process)

SHEV engines have a tendency for iterated intermittent steady-state engine operation at a specific high-efficiency point and engine stop. Consequently, this study focused on following two states in constructing a catalyst model at **the time of engine restart** when the air-fuel ratio changes dynamically (λ), and in **the period from a cold start to the completion of the light-off process** which has been an ongoing issue.

Then, based on the results of model gas experiments, we investigated the purification reaction properties of TWC, focusing mainly on the light-off tests under preset conditions of varying lambda at engine restart. From these results, we selected a total of 33 reactions essential for the reproduction of emission gas purification behavior at light-off and engine restart, including NH_3 and N_2O generation and decomposition, and constructed the basic form of the emission purification reaction model.

Next, based on the results of the light-off experiment, we identified the kinetic parameters with varying λ (at eleven different λ range between 0.88 and 1.03) and determined that the parameters change significantly at the rich (λ＜1) and lean (λ＞1) sides due to redox of catalyst surface. By **introducing a control method to produce changes in kinetic parameters for varying λ**, it is now **possible to reproduce the purification behaviour at engine restar**t. (Fig. 1)

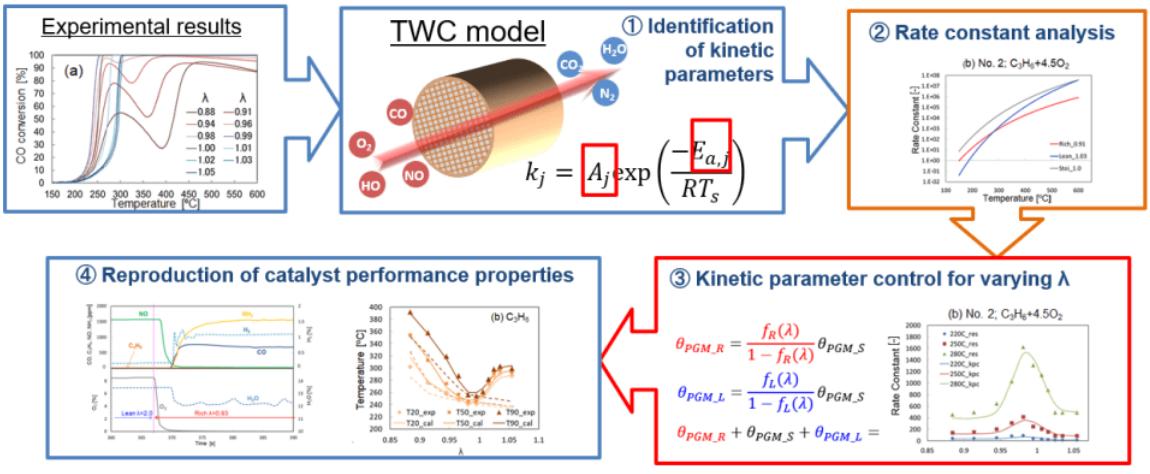

Figure 1. TWC model construction process introducing kinetic parameters for varying λ

Next, we aimed to reproduce the emission gas purification performance behavior at cold start, which requires the highest prediction accuracy. First, we conducted model gas light-off experiments with various pretreatment conditions. From the results, we found that catalyst surface of the rhodium layer, which was pretreated by exposure to an oxidative atmosphere, was oxidized and caused activation deterioration. We built a single-layer model reproducing the respective purification properties of the palladium layer and rhodium layer of the TWC, and for the activation behavior of the rhodium layer changing from the “Oxide base” (the initial deteriorated state due to catalyst surface oxidation) to the “Metal base” (activated state) depending on temperatures and lambda was **modelled by introducing a rate equation with Arrhenius form** (Fig. 2). Lastly, we **constructed a two-layer catalyst model by combining both layers**.

The completed model **dramatically improved the prediction accuracy in the challenging environment including the period from cold start to the completion of light-off**, and also gained the **capability for comprehensive estimation including NH_3 and N_2O emissions** (Fig. 3).

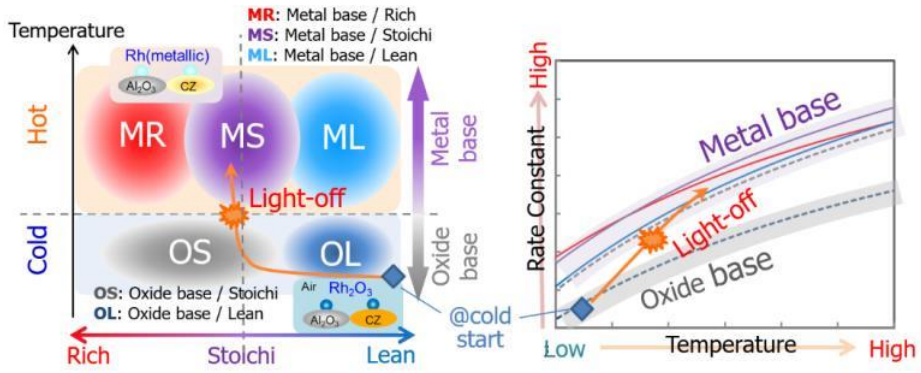

Figure 2. Concept of activation model from cold start due to redox of Rh

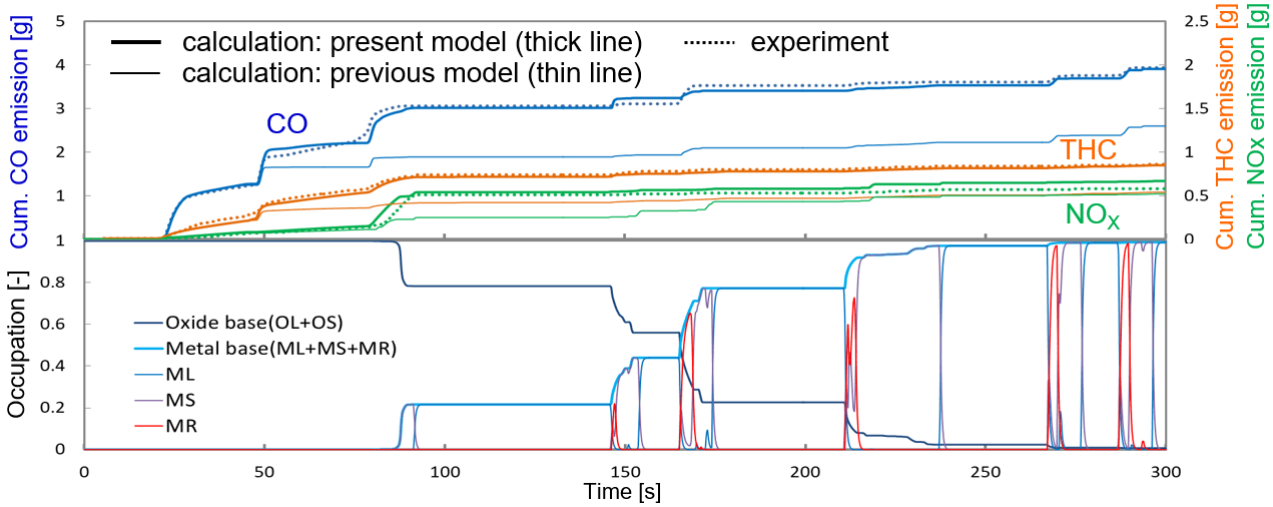

Figure 3. Cumulative emission amounts in WLTC mode simulation
and changes in activation states in the reaction model

Related papers:
Ind. Eng. Chem. Res. 2021, 60, 4, 1583–1601. (DOI: 10.1021/acs.iecr.0c05436)
Ind. Eng. Chem. Res. 2021, 60, 39, 14069–14086. (DOI: 10.1021/acs.iecr.1c02252)

■ About Catalyst Manufacturers Association, Japan (CMAJ)

Catalyst Manufacturers Association, Japan (CMAJ) is a non-profit industry association which was founded to stimulate the cooperation, communication, and interchange among its members and to promote the sound development of the Japanese catalyst industry. The membership comprises catalyst manufacturers, suppliers of catalyst-related materials, and companies engaged in the sales of catalyst products and materials.

■ About N.E. CHEMCAT CORPORATION

N.E. CHEMCAT CORPORATION is engaged in the development, manufacturing, and distribution of chemical catalysts, auto exhaust catalysts (including three-way catalysts and diesel auto catalysts), and fuel cell catalysts, and collection/refinement of precious metal catalysts.

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