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Estimation of hydrogen and oxygen concentrations in gasoline engine exhaust gas using FTIR analysis

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The Fourier transform infrared spectroscopy (FTIR) is possible to measure simultaneously multicomponent of gas and the main exhaust gas components of internal combustion engines except for total hydrocarbons (THC), hydrogen (H_2), oxygen (O_2) and nitrogen (N_2). In this study, the quantitative estimation methods are examined for H_2 and O_2 concentrations using FTIR and machine learning, though FTIR could not measure those species directly. About hydrogen, oxygen each, two kinds of method are evaluated in reference to a principle of the element balance. One is a method to regress from the correlation with the measurable gas components in FTIR analysis and the other is one using the infrared absorption spectrum. A partial least square regression (PLSR) and LASSO regression (LASSO-c) are adopted to the gas component-based models, and a LASSO regression (LASSO-s) to the absorption spectrum. The reference gas components are CO, CO_2, H_2O, NO and THC in the component regressions. A water gas shift reaction regression (SRR) model with a mean equilibrium reaction constant is also tested in the H_2 predictions. These are compared and validated in gasoline engine out exhaust gas emissions.

A 1.6 L inline four-cylinder turbocharged gasoline engine was used for the measurement. The engine-out exhaust gas was sampled upstream of a front catalyst converter and measured using a FTIR, a hydrogen mass spectroscopy, a magnetic pressure type oxygen analyzer and a flame ionization detector. The experiments were conducted under 24 steady-state operation points, the WLTC mode simulations both of warm and cold starts, and a real drive simulation. The experiment varying air-fuel (A/F) ratio 13.2 to 15.2 at 1500 rpm steady-state operation was also conducted.

The results of WLTC cold simulated operation was employed as training data.

On the prediction accuracy of the H_2 concentration, the regression using the spectrum, LASSO-s gives the best results in four models both for the transient cycles and steady-state operations as shown in Fig.1. The root mean square errors are less than 0.03 vol% and the coefficients of determination are more than 0.95. The reason why the spectrum regression is better is that a spectrum is more direct data and the model flexibility is also higher than those of the component regressions.

The H_2 concentration decreases monotonically for A/F ratio increasing. The differences between measurement and models are smaller on the lean side, while enlarged on the rich side. These conditions deviating from stoichiometry is out of the learning data range so that the results show a difference of the extrapolation prediction ability of the models. Moreover, the regression models reproduce a delicate change of the H_2 concentration according to A/F ratio variation depending on stoichiometric operation control.

The regression using the spectrum is better than others on the O_2 concentration estimation likewise as shown in Fig.2. In case of component regression, the difference with the measurement values of PLSR is smaller than that of LASSO. The difference between H_2 and O_2 models in this properties is thought to be caused from the data sensitivity characteristics that the water gas shift reaction namely dependence on CO is dominant in the H_2 regression, while the contribution of each component is comparable to the O_2 regression.

The transient responsivity of the models is the same as that of FTIR and can capture the concentration changes of H_2 and O_2 at the transient operating conditions well.

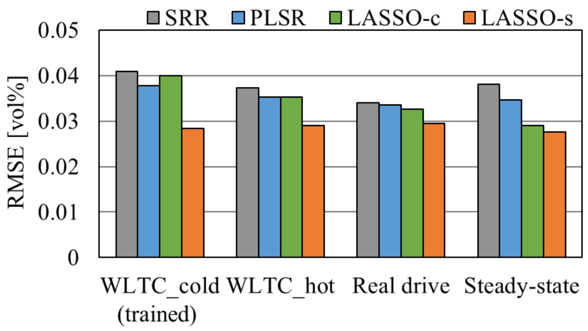

Fig.1 Comparisons of H_2 regression model accuracies

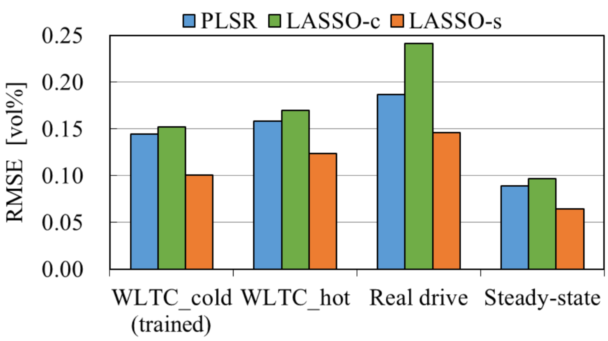

Fig.2 Comparisons of O_2 regression model accuracies

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