Activity function for predicting TWC performance as function of noble metal loading and catalyst mileage

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The development of a kinetic model describing the alteration of the TWC performance with respect to the catalyst noble metal loading and mileage (time-on-stream) has been a long-lasting task in automotive reaction engineering. Moreover, the sintering of PGM in TWCs has been widely regarded as the dominant factor for the deactivation of TWCs under real driving conditions typically operating above 650 °C. In this connection, it is highly desirable to develop a more robust methodology of model predictions based on the catalytic kinetics and physicochemical characteristics of TWCs. In the present study, 3D activity functions for each Pd and Rh catalyst have been independently developed on the basis of the active metal surface area (MSA) of Pd or Rh, respectively, which can be used to predict the TWC performance as a function of Pd or Rh loadings and the catalyst mileage. Consequently, the overall reaction kinetics for the double-layered Pd/Rh TWC monolith reactor as a function of the catalyst metal loadings and mileage has been derived by incorporating the activity functions developed for the Pd and Rh catalysts into the detailed reaction kinetics of the reference Pd and Rh catalysts.