Investigation of Gas Transport Properties on Urea Gas Decomposition Process in an SCR Monolith Reactor Using Computational Fluid Dynamics

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The urea gas decomposition is an essential process when applying the urea-SCR system to reduce NO_x emissions in combustion devices. It is difficult to examine directly a urea gas decomposition process in experiment when a urea solution is reacted with exhaust emissions. In this study, the single square channel monolith reactor is selected as an analytical domain to investigate the urea gas decomposition process by using a three-dimensional modeling. The purpose of this study is to find the gas transport properties that exert the strongest influence on the urea gas decomposition process in a single square channel monolith by comparing the simulation results of temperature-dependent gas transport properties with the constant ones. The processes in the gas phase, washcoat layer and solid substrate are simultaneously investigated by the assumptions of laminar flow and viscous gas at a steady-state. The simulations are varied with the combination of all constant gas transport properties, only temperature-dependent ones of density, diffusivity, thermal conductivity, specific heat and viscosity, and all temperature-dependent ones. The reactor performances are calculated and compared with the experimental ones at high and low temperature ranges.

The process of NO conversion in a urea-SCR monolith reactor system requires the NH_3 gas which is produced from the urea gas decomposition. In the numerical analysis of urea gas decomposition process, consequently, the NH_3 gas obtained by the calculation will influence the NO conversion and NH_3 oxidation. As the temperature increases, the values of gas transport properties such as viscosity, molecular diffusivity, conductivity and specific heat also increase, but in the contrary the density is decreased. The temperature-dependent one of density has a strong influence on the production of NH_3 gas in urea gas decomposition process. The molecular diffusivity has stronger influence at high temperature ranges compared to the density. From the simulation results it is shown that the gas transport properties with the strongest influence on the urea gas decomposition process in a single square channel monolith are the density and molecular diffusivity.

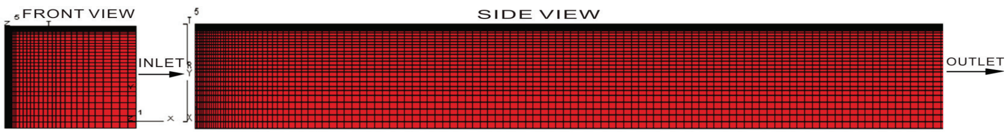

Fig. 1 Single grid configurations

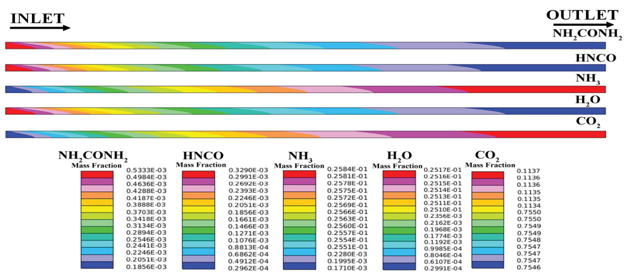

Fig. 2 Contour plots of NH_2CONH_2, HNCO, NH_3, H_2O and CO_2 species for the simulation with temperature-dependent gas transport properties at the cross-sectional view of y = 0 and the temperature of 523 K

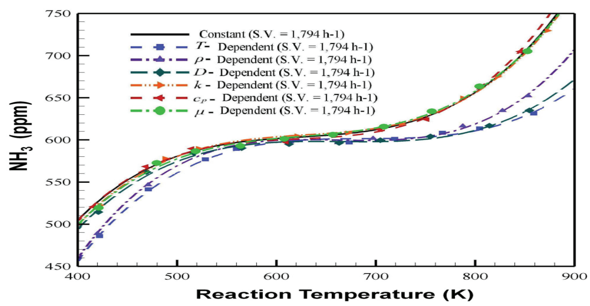

Fig. 3 Comparison of NH_3 concentrations in the outlet between the simulations with the various gas transport properties on the urea gas decomposition process at the different reaction temperatures

References

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