Kaew-arpha Thavornprasert 2010: Effect of Non-Uniform Temperature Distribution in a One-Zone TAP Reactor on Accuracy of Estimated Gas Diffusivities and First Order Irreversible Reaction Rate Constants. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Associate Professor Phungphai Phanawadee, D.Sc. 95 pages.

The TAP transient pulse response experiment has been increasingly used for heterogeneous catalytic reaction studies. The size and shape of the TAP response contain information on gas transport and chemical kinetics. Estimation of transport and kinetic parameters from the experimental response requires mathematical models describing the processes in the TAP reactor. The models are typically based on the assumption of uniform temperature distribution in the reactor. In this work, the effect of non-uniform temperature distribution in a one-zone reactor on the accuracy of estimated diffusivities and first order irreversible reaction rate constants are theoretically investigated via simulation for non-porous catalyst pellets. The experimental responses are obtained from simulation under non-uniform temperature distribution condition. Parameter estimation is performed using the uniform temperature distribution model. Estimation methods involve both the curve fitting (least-square) method and the moment-based method applied to different types of responses including exit flow rate curves and normalized responses. Deviations of estimated parameters from real values when using different methods are compared. Simulation results show that the deviations of estimated diffusivities are not larger than 0.62% indicating that the uniform temperature distribution assumption is valid for estimation of diffusivities. The deviations of estimated reaction rate constant can be large and depend on the estimation methods. Percentage deviations of estimated reaction rate constants obtained from the curve fitting of exit flow rates are generally smaller than those from other methods. For all estimation methods, the deviations of estimated reaction rate constants increase with increasing activation energy but decrease with increasing reactor temperature.

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