Satreerat Rueangrittiwong 2010: Effect of Assumption of Equal Gas Diffusivity Coefficient in All Zones in a Three-zone TAP Reactor on the Accuracy of Estimated Rate Constant. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Associate Professor Phungphi Phanawadee, D.Sc. 99 pages.

The experimental data from a TAP experiment is a response curve whose intensity is proportional to the exit gas flow rate. The response curve is used for estimation of the gas diffusivity and reaction rate constant. A three-zone TAP reactor usually applied in the TAP experiment contains a catalyst zone sandwitched between two inert zones. The gas diffusivity in each zone depends on the size and type of particles. An assumption of equal gas diffusivity in all zones would ease estimation of the reaction rate constant. The effect of assumption of equal gas diffusivity in all zones in the three-zone TAP reactor on accuracy of the estimated reaction rate constant was studied in this work by numerical simulation. The reaction rate constant was estimated by 3 methods including exit flow rate curve fitting, unit area normalized exit flow rate curve fitting and a calculation by the conversion expression. It was found that an accurate estimated reaction rate constant is obtained when the catalyst bed is thin, the gas conversion is low and the ratio of the gas diffusivity in the inert bed to that in the catalyst bed is close to unity. When the ratio of the length of the catalyst bed to the length of the reactor is 1/30 and the ratio of the gas diffusivity in the inert zone to that in the catalyst zone ranges from 0.667 to 1.333, the error of estimated reaction rate constant is less than 2% when the gas conversion ranges from 0.10 to 0.50 for all the estimated methods.

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