# A study on the dynamic modeling of a catalytic fixed-bed reactor adding numerical approximation of reaction effectiveness factor

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The purpose of this study is to improve the accuracy of the simulation results previously produced by the dynamic modeling method of catalytic fixed-bed reactor. The model is applied to the calculation of production of DME (dimethyl-ether) with the direct DME synthesis method. Dynamic modeling of catalytic fixed bed reactor is complicated for the general chemical reaction equations involve heterogeneous mass transfer schemes and Langmuir-Hinshelwood isotherm theory. Existing simulation methods on fixed-bed reactor for direct DME synthesis were focused on the steady-state modeling; therefore it could not deal with the result of inlet disturbances or addition of dynamic control algorithm. Assumptions such as regarding the reactor system as being in homogeneous phase were made to avoid ill-conditioning on numerical integration. Such simplification could be the main cause of the high conversion of feed material from the simulation than the actual demo plant data. To minimize the discrepancy between the simulation and experimental data, a numerical method is suggested to approximate the diffusion and reaction efficiency inside catalyst pellet at steady state.