Kinetic Analysis of H₂S Removal over several Mesoporous Metal Mixed oxides during Hot Coal Gas Desulfurization in a fixed-bed reactor Using the Deactivation Kinetics Model

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In 2014, the deactivation kinetics model (DKM) over mesoporous LaFeO₃/MCM-41 sorbents for hot coal gas desulfurization was established, which consisted of both the spatial and the time partial differential equations. The kinetic model can be used successfully to predict the distributions of H₂S concentration at different times and spatial positions with in fixed-bed layers, it is of very great significance to obtain basical chemical engineering data for the design of new reactor. For 50%LF₂ LaFeO₃/MCM-41 sorbent, the calculated apparent activation energy ($E_a$) and deactivation energy ($E_d$) for chemical reaction of LaFeO₃ active sites are 32.1 and 15.1 $kJ \cdot mol^{-1}$, respectively.

Using this DKM in 2017, the reaction order of each species was estimated for H₂S removal over mesoporous Cu–Mn mixed oxide/SBA-15 and La–Mn mixed oxide/KIT-6 sorbents. The reaction orders, rate constants, apparent activation energy ($E_a$), and deactivation energy ($E_d$) were calculated as the kinetic parameters. The calculated reaction orders, $\alpha$, $\beta$, and $\gamma$, were 1, 1, and 1 for Cu–Mn mixed oxide/SBA-15 and 0.6, 1.2, and 1 for La–Mn mixed oxide/KIT-6. The obtained $E_a$ and $E_d$ for Cu₃Mn₉ mixed oxide/SBA-15 were 33.02 and 46.34 $kJ \cdot mol^{-1}$ and for La₃Mn₉₇ mixed oxide/KIT-6 were 48.98 and 56.10 $kJ \cdot mol^{-1}$, respectively.

DKM has not considered the detailed characteristic parameters of the solid sorbent in such a microscopic way as unreacted shrinking core model (SCM) or general regression model (GRM) but in a macroscopic way. Therefore, DKM can be extensively applied to the kinetic analysis of noncatalytic heterogeneous reaction or adsorption processes without the requirement of structural property for sorbents.
