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Necessity of accurate and precise estimation of homogeneous surface diffusion model parameters for adsorption process

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Batch adsorption kinetics based on homogeneous surface diffusion model (HSDM) for phenol adsorption onto activated carbon is studied. Film mass transfer coefficient kc and the surface diffusion coefficient DS is estimated by finding the parameters using which the HSDM simulation gives a concentration profile which has minimum deviation with the experimental concentration time data. The deviation being minimized is the sum of square of error (SSE) between the simulated and experimental concentration-time data. Two of the traditional optimization techniques which are used widely for parameter estimations were used namely, Nelder Mead simplex algorithm (NMA) and Particle swarm optimization (PSO). kc and DS¬ values for runs with different initial concentrations, dosages and agitation were estimated. The variability in the estimated parameters and their implications were analyzed. Error surfaces were plotted by varying kc and DS values and plotting them against the corresponding SSE. Error surface analysis supported the need of approaching global minimum as the surface plotted had multiple optimum values. Time of operation required for 95% reduction of solute concentration in liquid from its initial concentration estimated based on parameters was studied. It was seen clearly that though the parameters fit the experimental data in an appreciable manner on observation, even the minutest fluctuation in them resulted in increasing the time of operation by up to 100% in some cases.

Biography

Akhil Gopinath has completed his Bachelor of Technology from Government Engineering College, Calicut and is currently pursuing MS in Chemical Engineering from Indian Institute of Technology Madras. He works in the field of modelling and simulation of adsorption processes and optimizing their performance.

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