Optimal distribution of catalyst in porous pellets for a quasi-steady-state reaction with Langmuir-Hinshelwood kinetics

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The conditions for enhancing the performance of a porous catalyst granule with a controlled activity profile are investigated for a catalytic reaction with Langmuir-Hinshelwood kinetics. The nonisothermal reaction and diffusion in the pellets with spherical, cylindrical, and planar shapes are studied, considering the presence of external mass and heat transfer resistances. The objectives of this paper are to investigate the influence of kinetic parameters on the productivity of the catalyst pellet, to find the optimal distribution of active catalyst in a porous pellet in the quasi-steady-state nonisothermal reactions, and to determine the main trends and dependencies by varying the parameters, such as Biot numbers, Thiele modulus, etc .

The mathematical models for chemical reactions with diffusion and non-uniform activity distribution in porous catalyst pellets were derived and analyzed. The maximum productivity (or effectiveness factor) can be achieved by expressing the distribution of active catalyst as Dirac δ -function. Due to the fact that the δ -function activity profile can only be considered theoretically, the Gaussian activity distribution was also studied.

As a result, the optimal position of the Dirac δ - function for productivity maximization was found. Then, the range of values of step-size, Biot numbers, and Thiele modulus for which the Gaussian productivity is close to the δ - function was obtained.

The parametric study leads to the conclusion that the higher productivity of porous catalyst pellets can be reached with non-uniform activity distribution in a quasi-steady state rather than with a steady-state uniform case. In addition, extremal control analysis was performed based on Lagrange equations, and such controlled profiles give the minimum value of productivity, while all the profiles other than that will result in greater productivity.

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