

Critical Thiele Modulus for Diffusion-Reaction Problems in Catalyst Slabs With Generalized Langmuir-Hinshelwood Kinetics

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The conditions for the occurrence of dead-core solutions to the nonlinear diffusion-reaction equation in catalyst slabs involving the generalized Langmuir-Hinshelwood reaction kinetics with reaction exponent of fractional order are derived analytically. The formation of dead zones where the reactant concentration vanishes is characterized by the critical Thiele modulus. Its approximations and exact value are derived as functions of the reaction exponent and the model parameter. The comparison principle theorem is formulated and proven to establish upper and lower bounds for the exact critical Thiele modulus. The effects of the reaction exponent and model parameter on the analytic approximations of the critical Thiele modulus, and dead-zone formation in catalyst slabs are analyzed. The critical Thiele modulus for problems with the generalized Langmuir-Hinshelwood kinetics and zero reaction exponent is derived explicitly, and profiles of critical solutions to the models with the generalized Langmuir-Hinshelwood and power-law kinetics are compared. Furthermore, a simple method to compute the dead-zone length and dead-core solutions is presented for problems with general reaction kinetics that admits dead-zone formation. Analytical results are illustrated numerically. The proposed analytical approach yields closed-form solutions for the critical Thiele modulus, offering valuable insights into the effects of process and model parameters on the formation of dead zones within catalyst slabs.

Słowa kluczowe

catalyst slabs, critical Thiele modulus, dead zone, generalized Langmuir-Hinshelwood kinetics, nonlinear diffusion-reaction equation

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