

Abstract: We investigate a nonlinear reaction-diffusion system coupled with convection-diffusion system. This combined system corresponds to physical description of heterogeneous catalysis when the flow of bulk-constituents is driven by a given stationary velocity field; diverse mechanisms between bulk- and surface-parts of the model-domain are described by Langmuir-Hinshelwood absorption kinetics; and the irreversible reactions on the catalytic walls meets the law of mass action with quadratic rate. The first part of the thesis is focused on analytical results; in Chapter 2 we prove existence and uniqueness of a mild solution for so-called near-by problem using nonlinear semigroup theory; in Chapter 3 we investigate the weak formulation of the problem. We prove an existence of a weak solution for little modified problem which, under an assumption, coincides with the original problem. In the second part of the thesis (Chapter 4) we numerically investigate the evolution of the bio-diesel microreactor. We compute numerical solutions using several methods and we test the results by analytical and physical conditions; with the aim to find the most efficient way to compute precise and physically correct solution.

Keywords: heterogeneous catalysis, coupled reaction-diffusion/convection-diffusion system, nonlinear semigroup theory, weak solution, bio-diesel microreactors