

Mass transport through dense, polymeric, catalytic membrane layer with dispersed catalyst

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The catalytic membrane reactor is widely recommended to apply for heterogeneous reactions. This reactor with segregated feed of reactant(s), and/or with separation of products improves safety, selectivity and efficiency of the catalytic processes. Thus, the hydrogenation, dehydrogenation, oxidation reactions, with different membranes, are the most common examples of the conversion enhancement [1, 2]. The catalytically active particles, as metallic complexes, activated carbon or metallic clusters, are commonly dispersed throughout the membrane phase as zeolite or polymeric material.

For description of this catalytic process a simple physical model was used for the membrane reactor as it is illustrated in papers [3, 4]. The cubic [3, 4], catalyst particles are uniformly distributed in the polymer membrane matrix. The diffusion paths are perpendicular to the interface and it takes place alternatively through membrane phase and catalyst particle. The reagent(s) diffuse(s) through the membrane, from its interface, into the first catalyst particle and then through the first particle into the membrane matrix, on the other side of the first particle and then to the second particle and so on through the whole membrane layer. In the present work, one dimensional, mathematical models have been developed for description of the mass transport through the membrane layer, taking into account the transport through the both phases and the chemical reaction, as well. The main assumptions of this model: process is steady-state; catalyst particle are cubic [3, 4] and uniformly distributed as well as they have uniform size; diffusion is perpendicular to the membrane interface; chemical reaction takes place in the catalyst particle; the diffusivities and the sorption coefficients are constants or concentration dependents.

Mathematical equations, given in closed form, were developed (similarly to that of three phase mass transfer [4, 5]), for description of the concentration distribution and the mass transfer rate at the interface, solving a differential equation system (containing $2N+1$ second-order differential equations, where N is the number of particles in the layer perpendicular to its interface; N can be a large integer number), in the case of first-order chemical reaction. The external mass transfer resistances are also taken into account. It will be discussed the effect of the ratio of diffusion coefficients in both the membrane matrix and catalyst particles, reaction rate constant, adsorption coefficient (for constant value as well as in the case of Langmuir adsorption isotherms), membrane thickness, external mass transfer coefficients. As a case study we discuss the reaction of alkene epoxidation with peroxide in a catalytic membrane reactor [3, 6].

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