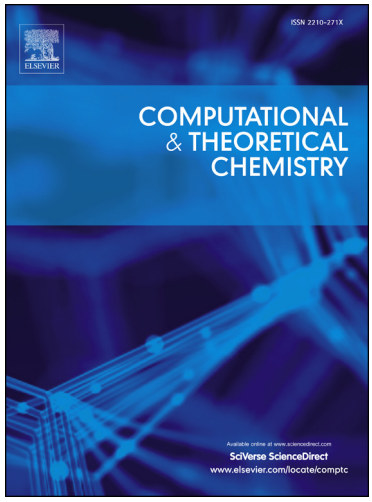

Computational study of the dimer-trimer and trimer-trimer reactions on the supported catalysts

Vladas Skakauskas, Pranas Katauskis

PII: S2210-271X(15)00317-5
DOI: http://dx.doi.org/10.1016/j.comptc.2015.08.002
Reference: COMPTC 1898

To appear in: *Computational & Theoretical Chemistry*

Received Date: 18 June 2015

Please cite this article as: V. Skakauskas, P. Katauskis, Computational study of the dimer-trimer and trimer-trimer reactions on the supported catalysts, *Computational & Theoretical Chemistry* (2015), doi: http://dx.doi.org/10.1016/j.comptc.2015.08.002

Computational study of the dimer-trimer and trimer-trimer reactions on the supported catalysts

Vladas Skakauskas*, Pranas Katauskis

Faculty of Mathematics and Informatics, Vilnius University, Naugarduko 24, 03225 Vilnius, Lithuania

Abstract

The kinetics of the dimer-trimer and trimer-trimer reactions, $nA_m + mB_n \to mnAB$ with $m = 2, n = 3$ and $n = m = 3$ proceeding on the composite (supported) catalysts is studied numerically by employing a phenomenological model which includes: the bulk diffusion of reactants from a bounded vessel towards the adsorbent and the product bulk one from the catalyst surface into the same vessel, adsorption and desorption of particles of both reactants, and surface diffusion of adsorbed molecules. Three different arrangements of the adsorption sites were used: the same concentrations of active and inactive sites and two different arrangements with equal total amount of the active and inactive in the reaction adsorption sites. Two adsorption cases of both reactants are considered: (i) each reactant adsorbs on both active and inactive sites, (ii) both reactants adsorb only on the support. Simulations of the mean-field model were performed using the finite difference technique. The influence of the size of the catalytic particle, surface diffusivity, and particle jumping rate constants via the catalyst-support interface on the catalytic reactivity of the supported catalyst is studied.

Key words: heterogeneous reactions, adsorption, desorption, surface diffusion, spillover

*Corresponding author. Faculty of Mathematics and Informatics, Vilnius University, Naugarduko 24, 03225 Vilnius, Lithuania. E-mail address: vladas.skakauskas@mif.vu.lt. Tel.: +370-5-2193084; Fax: +370-5-2151585.