



## Monte Carlo Simulation of Reaction-Diffusion of Chromium in Soil

S. Vito<sup>1,\*</sup>, M. Ifti<sup>2</sup>

<sup>1</sup>*University of Tirana, Faculty of Natural Sciences, Department of Industrial Chemistry;*

<sup>2</sup>*University of Tirana, Faculty of Natural Sciences, Department of Physics*

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**Abstract:** In this paper are presented results of Monte Carlo simulations of reaction-diffusion phenomena in soil, and they are compared with the experimental results of column adsorption of Cr(VI) solution. The experiment was performed under saturated steady state flow conditions. The system was studied for different flow velocities and initial concentrations. In all cases experimental breakthrough curves were obtained. The model used for Monte Carlo simulations of this process takes into consideration diffusion, as well as entrapment/detrapment processes. Entrapment and detrapment could be an adsorption/desorption or a reversible chemical reaction. Monte Carlo simulations of the model give very good agreement with the experimental results, obtained from experiments of column adsorption. Probabilities of diffusion, entrapment and detrapment that ensure the agreement of experimental and simulation results have been determined. Entrapment and detrapment probabilities make the difference between the cases. Hence these are the processes that determine the dynamics of the overall process.

**Key words:** *numerical model, transport process, Monte Carlo method, breakthrough curves, Cr (VI).*

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\* Corresponding: Email: [sonila.vito@fshn.edu.al](mailto:sonila.vito@fshn.edu.al); Tel: 00355672754817;