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**GRAND CANONICAL MONTE CARLO SIMULATIONS OF SORPTION EQUILIBRIA IN SILICALITE-1 TYPE ZEOLITE: APPLICATION TO HYDROCARBONS.** ***Sabrina Pricl****, Maurizio Fermeglia, and Massimo Simonetta, Department of Chemical Engineering, University of Trieste, Piazzale Europa 1, Trieste 34127, Italy, Fax: 0039-040-569823, sabrinap@dicamp.units.it*

Molecular simulations are an effective and complementary tool for studying the sorption thermodynamics of zeolitic systems. In particular, Grand Canonical Monte Carlo (GCMC) techniques are well suited for this purpose. In this work we performed GCMC simulations of sorption equilibria of methane, ethane, propane, butane, hexane, cyclohexane, benzene and toluene in a silicate-1 type zeolite. The results obtained show good agreement with the corresponding experimentally available sorption isotherms and isosteric heats. Further, they indicate that the considered hydrocarbons behave ideally within the zeolite pores, and that each species prefers to locate at different positions within the zeolite pore framework, in harmony with theoretical predictions.