Abstract Submitted for the MAR14 Meeting of The American Physical Society

Gas Adsorption Kinetics in Pores: A Computer Simulation Study¹ RAMNATH SELAGAMSETTY, M. MERCEDES CALBI, Physics & Astronomy, University of Denver — We present results for the kinetics of adsorption of a gas inside a cylindrical pore. The study is based on a Kinetic Monte Carlo simulation performed on a lattice that includes a central line of sites encircled by a cylindrical shell of sites. We monitor the time evolution of the overall coverage as well as its distribution along the pore. We also keep track of the transfer of particles between the two groups of sites and analyze its consequences on the equilibration time of the system. We compare the resulting dynamics with the one observed for narrower pores where a single line of sites is considered.

¹Work supported by NSF through grant CBET-0746029.

Maria Calbi University of Denver

Date submitted: 14 Nov 2013 Electronic form version 1.4