

Continuous-Time Random Walk Simulation of Surface Kinetics

Q. Chang¹, E. Herbst²

¹Department of Physics, The Ohio State University, Columbus, OH 43210, USA
email: chang.442@osu.edu

²Departments of Physics, Chemistry and Astronomy, The Ohio State University, Columbus,
OH 43210, USA

Abstract.

The continuous-time random walk (CTRW) Monte Carlo method has been proven to be an accurate and powerful method to simulate surface kinetics. This method can be used no matter how complex a surface is; thus, it provides a good tool to simulate interstellar grain-surface chemistry. We used the CTRW Monte Carlo approach to study a moderately complex network of diffusive reactions occurring on interstellar grain surfaces. The chemistry starts as H, O and CO species from the gas adsorb onto dust particles and leads to the production of species as complex as methanol. We first performed the simulation on a pure olivine surface and then on various surfaces on which molecular hydrogen can be efficiently produced over a range of temperatures. We also simulated a surface on which an ice mantle is gradually developed, so that the kinetics are time-dependent. The goal of the study is to find out how more complex surfaces will affect surface chemistry.

Keywords: ISM: molecules, molecular processes
