A hybrid moment equation approach to gas-grain chemistry

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Complementary to the gas phase chemistry, chemical processes happening on the grain surfaces are important for the overall interstellar matter repository. Due to their discrete and stochastic nature, however, usually surface chemistry cannot be accurately modeled by the rate equations. Various methods have been proposed, including the modified rate equation approach (Caselli et al. 1998; Garrod 2008), master equation approach with cutoff (Stantcheva et al. 2002), moment equation approach with cutoff (Lipshtat and Biham 2003; Barzel and Biham 2007), multiplane approach (Barzel et al. 2007), and the exact Monte Carlo approach (Vasyunin et al. 2009). The Monte Carlo approach would produce the most accurate results if it is repeated for many times; however, it is computationally heavy, and eventually impractical when a large chemical network is being modeled. On the other hand, a consistent and automatic algorithm is needed to handle a generic system in which both the gas phase and grain surface processes are included. In the present work, we propose a moment equation approach in which the generating function machinery is used to generate the equations automatically (up to any prescribed order), and a cut-off-and-switch scheme is implemented to approximate the infinite system of equations. Comparisons are made between the results of this method and those from the exact Monte Carlo simulations for several commonly used systems. The agreement is usually satisfactory, while the speed of our method is not much slower than the rate equation approach. Further issues include the numerical stability of this method (when higher order moments are included), how to control the errors quantitatively, and how to select those mostly needed terms to limit the number of variables and lower the computational burden.

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