

A Hybrid Approach of Rate Equations and Moment Equations to Treat Gas-Grain Chemistry for Large Reaction Networks

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We present a hybrid approach of rate equations and moment equations to study large gas-grain chemical networks. Specifically, we build a time-dependent chemical model of the interstellar medium, which involves about 6000 gas-phase reactions and 300 grain-surface reactions. The evolution of the gas-phase chemistry is modeled with rate equations, as this method is computationally efficient. For the surface reactions, we still use rate equations when the either reactant is more abundant than one per grain; when the abundance of reactants is lower than one per grain, the stochastic effect must be taken into account and therefore we use moment equations developed by *Barzel and Biham*. The gas-phase and grain-surface are coupled via thermal desorption and accretion.

We compare the result of this hybrid method to the result of pure rate-equation method for our standard interstellar medium conditions. We found that at 10K, the hybrid method agrees well with the rate-equation approach up to 1 million years. We also discuss the differences at higher temperatures and smaller grain sizes.

Reference:

Barzel, B., & Biham, O. 2007, J. Chem. Phys., 127,144703