A GAS GRAIN MODEL OF INTERSTELLAR CLOUD CORES WITH MOMENT EQUATIONS TO TREAT SURFACE CHEMISTRY

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We have built a gas-grain model of homogeneous cold cloud cores with time-independent physical conditions. In this model, we use the full OSU gas phase network, which involves 458 gas phase species and more than 4000 reactions, and treat it by rate equations which is totally deterministic. A small surface reaction network accounts for the productions of stable molecules such as H_2O , CO, CO_2 , H_2CO , CH_3OH , NH_3 and CH_4 . The surface reactions are treated by a hybrid method of moment equations (Barzel & Biham 2007) and rate equations: when the abundance of a surface species is lower than a specific threshold, say one per grain, we use the stochastic moment equations to simulate the evolution; when its abundance goes above this threshold, we use the rate equations. A continuity technique is utilized to secure a smooth transition between these two methods.

We have run chemical simulations for a time up to 10^8 yr at three temperatures: 10 K, 15 K, and 20 K. The results will be compared with those generated from (1) a completely deterministic model that uses rate equations for both gas phase and grain surface chemistry, and (2) modified rate equations (Garrod 2008) that partially take into account the stochastic effect for surface reactions. At 10 K, our model results agree with the above two methods, while discrepancies appear at higher temperatures and smaller grain sizes.