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Gas-grain chemical modeling of dynamical dark cloud environments

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Abstract. Whilst many dark cloud chemical models exist, the vast majority deal exclusively with the gas phase component, or merely approximate the dust grain surface chemistry by fixing accretion rates to produce grain mantle abundances in line with expected values. However, surface chemistry is increasingly being invoked as a solution to the problems of gas phase-only models; methanol production in dark clouds may be a case in point.

The Ohio State University gas-grain code has been used for some years to model explicitly the reactions of grain surface-based species, to produce fully time-dependent coupled gas and grain chemistries. This has allowed consideration to be given to the physical processes which occur on dust grain surfaces, under physical conditions appropriate to the interstellar medium, and how these impact on gas phase abundances.

Previously the OSU code has been restricted to static dark clouds. This static case has been studied in many publications. We now introduce dynamics to the model, allowing for time- and depth-dependent density and visual extinction changes, as well as moderate temperature variations. The completion of the model to become a multi-point dynamical chemical code is particularly pertinent in the light of recent observational evidence of small-scale density structure in the ISM. Hence, we apply the code to a number of physical situations including: pre-stellar core collapse, hot cores, and transient dark cloud cores. We also introduce mechanisms for gas phase molecular self-shielding so that photodissociation regions may be modeled with this comprehensive approach.

Keywords: Astrochemistry, molecular abundance, ISM: cloud