Astrochemical modelling: Coupling physical and chemical properties of interstellar gas and dust

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Low-mass protostars form from the collapse of dense cores in clouds of molecular gas. In the very early stages, the protostar is deeply buried in an envelope of gas and dust. The material of the envelope is later accreted onto a protoplanetary disc around the protostar and onto the protostar itself. The molecular line emission from star-forming regions can be used to probe the physical characteristics of the region, both directly, through excitation analysis, and indirectly, through studies of the chemical reactions that form the observed molecules. Such an analysis heavily relies on inclusion of the reactions on the icy surfaces of interstellar dust grains, where e.g. hydrogenation reactions contribute to the formation of more complex molecules.

Our own Solar System is known to have formed in the presence of several massive stars – meteoritic evidence shows that short-lived radionuclides were injected from a nearby supernova explosion, or even multiple supernova events. It is therefore extremely important to investigate the influence of external effects on the chemistry of cores which can form low-mass protostars, like the Sun. Our previous observations show that increased temperatures resulting from the irradiation from nearby luminous stars have effects on the chemistry of the star-forming core due to evaporation of key species such as carbon monoxide and methane from the dust grains.

We here demonstrate the early results of our new time-dependent astrochemistry code which couples an advanced gas-chemistry code (based on the reactions in the UMIST database) with freeze-out and evaporation of molecules onto dust grains as well as grain-surface chemistry. The code also treats the temperatures of gas and dust separately, includes the relevant heating and cooling terms for both gas and dust (cosmic ray heating, spectral line cooling, UV irradiation, etc.), and couples the physical properties of gas and dust through gas-grain interactions.

With our code we have first studied how the chemistry of a dense dusty core is affected by a nearby supernova explosion, resulting in an increase in the cosmic-ray ionisation rate. The results from our code will be used to thoroughly investigate the impact supernovae have on the chemistry of star-forming regions, and be compared with observations of protostellar envelopes in supernova remnants. Ultimately, the code will help us to identify tracers showing the irradiation history of protostellar clouds.