

Simulating the chemistry and dynamics of molecular clouds

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Abstract. We have performed high-resolution three-dimensional simulations of turbulent interstellar gas that for the first time self-consistently follow its coupled thermal, chemical and dynamical evolution. Our simulations have allowed us to quantify the formation timescales for the most important molecules found in giant molecular clouds (H₂, CO), as well as their spatial distribution within the clouds. Our results are consistent with models in which molecular clouds form quickly, within 1–2 turbulent crossing times, and emphasize the crucial role of density inhomogeneities in determining the chemical structure of the clouds.

Keywords. astrochemistry – molecular processes – methods: numerical – ISM: clouds – ISM: molecules

One of the main difficulties involved in the numerical modelling of the formation and evolution of giant molecular clouds (GMCs) is the fact that their chemical, thermal and dynamical evolution is strongly coupled. Prior attempts to model GMCs have typically dealt with this problem with ignoring one or more aspects of this coupling, e.g. by assuming that the gas remains isothermal in hydrodynamical simulations. As a first step towards producing more realistic cloud models, we have developed a lightweight treatment of cloud chemistry and cooling that has allowed us to perform high-resolution three-dimensional simulations of turbulent interstellar gas that accurately model the gas chemistry, cooling, and the hydrodynamics. Full details of this treatment and of the simulations that we have performed can be found in Glover *et al.* (2009). In this contribution, we restrict ourselves to highlighting a few of our most important results.

We find that CO formation occurs rapidly in dense, turbulent gas. Most of the CO in our simulations forms within the first 1–2 turbulent crossing times, on a similar, but slightly slower timescale to the H₂. These short chemical timescales suggest that the limiting timescale in the formation of a GMC is not the time required to convert H to H₂ and C⁺ to CO, but rather the time required to assemble the cloud material from the low density ISM. We also find that the CO abundances produced in our simulations are highly inhomogeneous, and are not well correlated with either the local gas density or with the effective visual extinction. Instead, it appears to be a combination of these quantities that best predicts the resulting CO abundance. This has important consequences for attempts to infer the structure of real GMCs from observations of the CO emission.

References

Glover, S. C. O., Federrath, C., Mac Low, M.-M., & Klessen, R. S. 2009, *MNRAS*, in press; arXiv:0907.4081