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Erratum: The chemistry of transient molecular cloud cores

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ABSTRACT

We assume that some, but not all, of the structure observed in molecular clouds is associated with transient features which are not bound by self-gravity. We investigate the chemistry of a transient density fluctuation, with properties similar to those of a core within a molecular cloud. We run a multipoint chemical code through a core's condensation from a diffuse medium to its eventual dispersion, over a period of $\sim$1 Myr. The dynamical description adopted for our study is based on an understanding of a particular mechanism, involving slow-mode wave excitation, for transient structure formation which so far has been studied in detail only with plane-parallel models in which self-gravity has not been included. We find a significant enhancement of the chemical composition of the core material on its return to diffuse conditions, whilst the expansion of the core as it disperses moves this material out to large distances from the core centre. This process transports molecular species formed in the high-density regions out into the diffuse medium. Chemical enrichment of the cloud as a whole also occurs, as other cores of various sizes, life-spans and separations evolve throughout. Enrichment is strongly affected by freeze-out on to dust grains, which takes place in high-density, high visual extinction regions. As the core disperses after reaching its peak density and the visual extinction drops below a critical value, grain mantles are evaporated back into the gas phase, initiating more chemistry. The influence of the sizes, masses and cycle periods of cores will be large both for the level of chemical enrichment of a dark cloud and ultimately for the low-mass star formation rate. The cores in which stars form are almost certainly bound by their self-gravity and are not transient in the sense that the cores on which most of our study is focused are transient. Obviously, enrichment of the chemistry of low-density material will not take place if self-gravity prevents the re-expansion of a core. We also consider the case of a self-gravitating core, by holding its peak density conditions for a further 0.4 Myr. We find that the differences near the peak densities between transient and gravitationally bound cores are generally small, and the resultant column densities for objects near the peak densities do not provide definitive criteria for discriminating between transient and bound cores. However, increases in fractional abundances due to reinjection of mantle-borne species may provide a criterion for detection of a non-bound core.

Key words: errata, addenda – MHD – stars: formation – ISM: clouds – ISM: molecules.

The paper 'The chemistry of transient dense cores' was published in Mon. Not. R. Astron. Soc. **356**, 654–664 (2005). An incorrect version of the paper appeared in print: the published paper was not the final version. Hence the subsequently modified sections of the paper are being published in their entirety in this Erratum. Differences between the correct and incorrect version consist of the alternative title, a longer abstract, and some additions to the introduction and conclusions. However, none of the results, conclusions or general content printed previously were at fault. We also thank both referees.

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1 INTRODUCTION

A number of studies have identified small-scale density inhomogeneities in dark clouds (e.g. Girart et al. 2002; Morata, Girart & Estalella 2003). Morata et al. (2003) used the BIMA interferometer array to make observations of a dense condensation in the L673 region, in the molecular transitions of CS ($J = 2 \rightarrow 1$), N_2H^+ ($J = 1 \rightarrow 0$) and HCO^+ ($J = 1 \rightarrow 0$). The greater resolution provided by this instrument revealed a smaller-scale structure than previously seen with a single dish. Several cores of gas of size $\leqslant$0.08 pc were detected in each molecular line, most with the molecular line maxima displaced from each other. This suggested a heterogeneous medium of cores, of various densities and at various stages of chemical evolution.

Girart et al. (2002) carried out a molecular line survey of a dense quiescent core (scale of ∼0.1 pc) ahead of the Herbig–Haro object HH2, which showed an enhanced chemistry. The illumination of the core with an ultraviolet (UV) field emanating from the shocked region HH2, and the subsequent chemical enhancement, aided in its detection. Follow-up modelling work (see Viti et al. 2003) suggested that only a short period of time had passed since irradiation had commenced (∼100 yr), implying that the core's formation was not a result of the dynamical action of HH2. The models also indicated that the core had spent only a moderate period at high density (<2 Myr) before irradiation, which could indicate a transient nature for such objects.

In this paper, we postulate that molecular clouds are largely made up of assemblies of transient cores surrounded by a more diffuse medium from which they condense. Obviously the relationship between star formation and cores implies that self-gravity is important in some cores; cores bound by their self-gravity will not be transient in the sense that we are considering at least some of the cores to be transient.

Traditionally, core formation has been attributed to self-gravity (e.g. Fiedler & Mouschovias 1992; Ciolek & Mouschovias 1995). Self-gravity can induce core formation even in regions where the thermal and magnetic pressures are initially comparable (e.g. Balsara, Ward-Thompson & Crutcher 2001).

However, since the publication of the paper by Arons & Max (1975), many authors have considered the material from which molecular cores form to have initially low values of the thermal pressure to magnetic pressure ratio, β. As discussed by Falle & Hartquist (2002) (hereafter FH02), when this ratio is initially small the presence of waves with suprathermal amplitudes within the translucent clumps of giant molecular clouds leads to high-density, transient structures on many scales including those in which self-gravity is unimportant. The formation of high density contrast transient structure involves the excitation of slow-mode waves as a consequence of the non-linear steepening of fast-mode waves. The mechanism does not lead to much larger density contrasts than initially present unless the initial magnetic pressure is much larger than the initial thermal pressure. The numerical results in FH02 are for plane-parallel, time-dependent magnetohydrodynamic (MHD) models, designed to gain an understanding of the non-linear mechanism leading to the formation of structure with density contrasts in excess of 10. They are currently extending the work to more dimensions, and the mechanism that they have identified is no doubt important in existing multidimensional studies of core formation in magnetized media in which self-gravity has been included (e.g. Gammie et al. 2003). However, the inclusion of the self-gravity and the way in which the simulations have been analysed do not facilitate an examination of the importance of the mechanism discussed by FH02.

With the possibility in mind that at least some cores are not bound by their self-gravity and are transient, we attempt to simulate the chemistry of one of these cores as it evolves physically, over a characteristic time-scale of approximately one million years, with the main purpose of finding tracers for its evolution. This requires a description of the way in which cores form, evolve and eventually disperse, from the point of view of a parcel (or parcels) of gas within a core. FH02 conducted simulations of plane-parallel MHD waves passing through a cold plasma, and found that modest density perturbations could lead to the growth of significant density inhomogeneities. They produced a number of spatial density profiles, which, very broadly, showed an initially shallow-peaked function evolving into a sharp, strongly peaked function, gradually dying away again. Our Fig. 1 shows fig. 6(a) from FH02: spatial density profiles for three different times in the growth stage, $t = 3$, 3.5, 3.6×10^3. Units are determined according to parametrization of variables in FH02. Plots of the time evolution of the *peak density* showed another similarly peaked function.

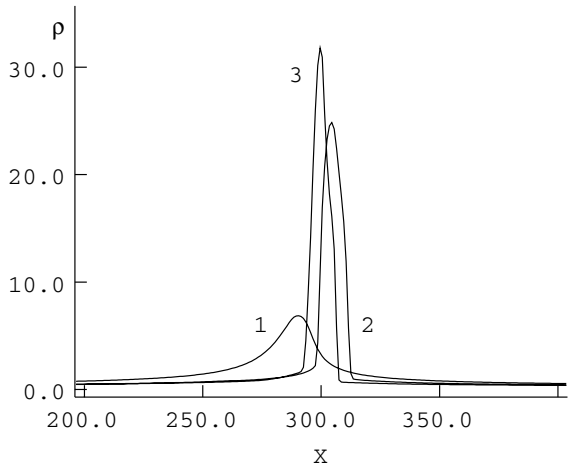

Figure 1. Density profiles at three different times in collapse phase, from fig. 6(a) of FH02.

In order to obtain a chemical description of the dense cores, we are required to make qualitative approximations to the density profiles of FH02, and use these in independent chemical codes. This is necessary since the construction of a coupled MHD–chemical code with which detailed chemical observations of dense structures can be explained is at present a long way off. Whilst in the FH02 simulations only one spatial variable is considered, this is the only work to address specifically the generation of structure in a low-β environment by the mechanism of slow-mode excitation in fast-mode shocks. Many multidimensional MHD simulations exist; however, almost all have been performed with codes based on non-conservative schemes. Falle (2002) has pointed out the difficulties with such codes for even very simple problems. Moreover, almost all such calculations either have followed the decay of artificially imposed velocity and density spectra or have included distributed source terms to drive 'turbulent' motions in a totally unphysical manner. In reality, the internal motions are driven by perturbations at the boundaries. Even in simple geometries, the construction of the boundaries and boundary conditions requires serious thought.

Hence, because the FH02 results are presently the most relevant to the picture that we are exploring, and because of the simulations' plane-parallel character and the non-linear, non-Alfvénic nature of the perturbations, we are restricted to a qualitative approach to the incorporation of their density profiles into a chemical model.

To do this, we here approximate them as Gaussians in space and time, which they resemble. We model the spatial density profile as a Gaussian whose scale varies with time. The central density of the core (to which the densities at all other points are referred) also follows a time-dependent Gaussian. The resulting space- and time-dependent Gaussian is constrained by the conservation of mass. No other hydrodynamic conservation equations (i.e. energy, momentum) are included. Rather, realistic time-scales and distances adopted for the collapse and expansion are specified. The space- and time-dependent visual extinction through the core is calculated as a function of density.

By simulating the chemistry of a core in this way, and focusing on a number of parcels of gas at positions from centre to edge, we

attempt to build up a picture of the entire core, to find chemical tracers of its evolution, and to describe the spatial behaviour of these tracers. This study may then provide a means by which to put some constraints on the ages and the evolution of physical and chemical conditions of actual cores. Further, we may illuminate the connection between the cores and the surrounding diffuse medium, and see how the transient cores act to enhance the overall chemical composition of a dark cloud. In this paper we test the hypothesis that cores are in a continual state of dynamical evolution, and we identify potential chemical diagnostics of such activity. In future work we will consider a cloud to be an assembly of such transient dense cores.

6 CONCLUSIONS

Self-gravity becomes important during at least some phases of the evolution of a core in which a star eventually forms. Self-gravity certainly prevents at least some cores from re-expanding without the input of momentum or energy from a young star. However, in regions in which the magnetic pressure is initially very large compared to the thermal pressure, high density contrast features, in which self-gravity is unimportant, can develop as a consequence of non-linear MHD processes. Such features are transient and some may be similar to some observed cores. While some cores in molecular clouds are bound by self-gravity and certainly are not transient in the sense that features in the simulations of FH02 are transient, some cores may be transient.

This is the first study of the chemistry in transient density inhomogeneities in molecular clouds, such as have been observed and are predicted in MHD calculations. The main premise of this work is that dark clouds possess non-uniform density structures, consisting in part of transient localized fluctuations (cores) within a diffuse background medium. Observational and computational evidence suggests that the chemistry of the cores is mostly young, of the order of 1 Myr, implying such a time-scale for their *physical* evolution (and destruction). As a result of the action of the interstellar radiation field, which should permeate strongly at least through the diffuse component, freeze-out should be limited to taking place only within the condensations. The importance of freeze-out in dark clouds would therefore be coupled to the cycles over which cores form and disperse, since the characteristic freeze-out time-scale is also of the order of 1 Myr. The cyclic evolution of cores should bring about some degree of transportation of material formed in high-density regions into the diffuse background medium. In a case where (at least locally) the evolution time, size of core, etc., are essentially the same, a 'limit cycle' may be reached, after which point the chemistry of the core will not change from cycle to cycle (see Nejad, Williams & Charnley 1990).

The results of this model also emphasize the need for multipoint chemical codes in modelling dense cores. The central fractional abundances are quite different from those abundances at greater distances from the core centre, particularly with respect to the crossover between freeze-out and non-freeze regions. The column densities that we should expect to observe through dense cores would not be solely dependent on the central fractional abundances, so we should not expect single-point simulations to match observations very well. A limited number of papers (e.g. Nejad et al. 1990; Nejad & Williams 1992; Charnley et al. 1988a,b) have considered chemistry in material that passes from lower density to higher density and then back to lower density conditions. However, the dynamical descriptions in those papers were adopted with a view to considering the effects of disruption by the winds of young stars. Furthermore, multipoint calculations allowing the determination of the spatial profiles of chemical abundances at multiple times have been adopted in none of the previous work involving the chemistry of material cycled between lower and higher and back to lower density states. As stated above, the current results demonstrate that multipoint calculations are required.

The results from this study yield a number of specific conclusions, as follows.

(i) The spatial extents of several key species (CO, N_2, H_2O and NH_3) are significantly enhanced by the cycling process, implying a source of general molecular enrichment of clouds.

(ii) The relative spatial extents of CS and NH_3 are broadly in agreement with the observed morphologies of star-forming regions.

(iii) The absolute values of the CO abundance are significantly higher than the values obtained for simple quasi-static collapse models. Such enhancements should be observationally detectable at the outer boundaries of translucent clumps. Many of the time- and space-dependences of the various chemical species are only detectable at high resolutions and cannot be resolved with single-dish telescopes.

(iv) Although the recycling of material frozen out on to dust grains results in instantaneous chemical enrichment of the gas, the chemical effects are not long-lived, although certain species will be strongly enhanced as a result, when averaged over time.

(v) Many species, mostly represented in Table 3, show enhancements at peak density of their integrated column density-calculated fractional abundances. Of those, the following are expected to be enhanced and remain significantly enhanced even after core re-expansion: CO, N_2, N_2H^+, NH_3, NO, CH_4, O_2, H_2O.

(vi) The dynamical turnover means that clouds that are ensembles of such transients have a clearly different chemistry from a 'traditional' static cloud. The reinjection of material from solid to gas that occurs as material passes through the $A_{V,\mathrm{crit}}$ zone during re-expansion is crucial for gas-phase chemistry. We have fixed our treatment with reference to observations. However, this work shows that the factors determining $A_{V,\mathrm{crit}}$ need to be much better determined than they are now (Williams, Hartquist & Whittet 1992).

(vii) Specific differences include the fact that the gas-phase chemistry is 'young' at all times if the turnover time is $\sim$1 Myr. A young chemistry is consistent with observations; a turnover time of $\sim$1 Myr is consistent with predictions from MHD. Secondly, freeze-out is important, obviously, but because of the turnover never goes to completion (i.e. 100 per cent freeze-out).

(viii) Transient clumps that happen to be denser and more massive than the average will have stronger gravitational fields that will dominate the MHD processes that tend to dissipate the clump. The critical case occurs when these tendencies are in near-balance, and the transient inhomogeneity may be expected to be near-static for a period. We have explored the chemistry in such a case; there are some differences from the gravity-free model, although these are probably not observationally significant. Therefore we have been unable to predict a clear signature of a 'hung' inhomogeneity. However, features resulting from the reinjection of mantle-bound species back into the gas phase may provide criteria for determining cores that are in a re-expansion phase of evolution, and therefore not in a bound, self-gravitating state. The strength of these features should depend on a number of poorly defined free parameters in our models.

(ix) Nevertheless, the model of a molecular cloud presented here has implicit within it the reason why the overall efficiency for low-mass star formation is rather small: the MHD forces dissipate most of the smaller clumps before collapse can occur. The low efficiency (a few per cent) must be related to the mass spectrum of the transient inhomogeneities, to be determined in an extension of the work of Falle & Hartquist (2002) in which three-dimensional structures are considered.

(x) A specific prediction of this model is that the background gas in which the inhomogeneities are embedded is fairly diffuse. It is, however, chemically enriched when compared to the chemistry of a canonical isolated static diffuse cloud model. These chemical enhancements may account for the variety of chemistries observed in diffuse clouds; this might occur when the line of sight towards a bright star passes through diffuse regions of a molecular cloud. Thus, this study of dynamical molecular clouds may also give some information about the place of diffuse clouds in the general scheme of interstellar circulation.

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