Hunt for Molecules
F. Combes, F. Casoli, E. Falgarone, L. Pagani (eds)

NON-EQUILIBRIUM CHEMISTRY IN THE COLD DIFFUSE INTERSTELLAR MEDIUM

Falgarone, E.[1], Hily-Blant, P.[2] and Pineau des Forêts, G.[3]

Abstract. A persistent problem of interstellar chemistry in cold diffuse gas is the integration of carbon and oxygen atoms in molecules. Elements of a reply are now provided by our understanding of turbulence and its intermittent dissipation. Observations at high spectral and spatial resolutions of HCO^+ and CO lines have been a guidance to outline the main features of the dissipative structures of turbulence in the cold diffuse medium and the chemical processes they trigger.

1 Introduction

Thirty years ago, new fields of molecular astrophysics were just opening and challenges were everywhere, driven by the detection of molecules with a new technique: the heterodyne detection extended into the range of microwaves. We were discovering at once an unsuspected cold universe with gas temperatures below 10 Kelvin (Penzias et al. 1972). It soon appeared that energetic sources were well hidden in the large masses of cold gas that we were observing: X-ray photons and high-velocity flows emitted by invisible sources were detected. These cold masses of gas happened to be the long-searched sites of star formation. In the mean time, the chemical processes invoked to identify many so-called unidentified features and understand the routes of

---

[1] LERMA/LRA, ENS & Observatoire de Paris, France
[2] IRAM, Grenoble, France
[3] IAS, Orsay, France

molecule formation have been continuously enriched by new experimental and theoretical data and accurately coupled to the physics of the gas. It is remarkable, though, that the resulting sophisticated models still fail at explaining some among the oldest puzzles raised by interstellar chemistry: the large observed abundance of CH^+ in diffuse gas or the origin of the diffuse interstellar bands.

To some extent, present is even more challenging. We are discovering the need to couple disciplines which have ignored one another in the past, at least in the field of astrophysics: chemistry, turbulence, dusty plasma physics, magnetic fields, physics of aggregates and nanoparticles, among others. We also start to couple gravity that drives the evolution of the universe to that of the dissipative baryonic matter.

These few pages are meant to illustrate these new challenges: it sets the stage for a very active diffuse interstellar medium (ISM), pervaded by a turbulent cascade that extends down to scales possibly as small as a few tens of AU, and whose dissipation is shown to able to trigger the first steps of gas-phase chemistry, inhibited in the cold diffuse ISM.

2 Warm glitters in the cold diffuse ISM

The diffuse ISM, long thought of as a mixture of phases in thermal pressure balance (McKee & Ostriker, 1977) is also turbulent, with supersonic, possibly superAlfvénic velocities. It houses the first steps of interstellar chemistry, recognized long ago by Watson (1974) and Black & Dalgarno (1977) as most challenging. For carbon and oxygen, the energy requirements are so high that they are highly inhibited in the cold ISM: the reaction $C^+ + H_2 \rightarrow CH^+ + H$ has an endothermicity $\Delta E/k = 4640$ K and $O + H_2 \rightarrow OH + H$ has an activation barrier $\Delta E/k = 2980$ K. These two critical steps are yet the only routes towards CH^+, HCO^+ (a daughter molecule of CH^+ in diffuse gas), OH and H_2O (a daughter molecule of OH). The large abundances observed in the diffuse medium of CH^+ (Crane, Lambert & Sheffer 1995, Gredel 1997), HCO^+ (Liszt & Lucas 1996; Lucas & Liszt 2000), and H_2O (Neufeld et al. 2002, Plume et al. 2004) cannot be explained by its known steady-state chemistry, driven by UV photons and cosmic rays. It has long been recognized that this chemistry has to tap non-thermal energy reservoirs of the ISM, such as magneto-hydrodynamical (MHD) shocks (Elitzur & Watson 1980, for a review see Scalo & Elmegreen 2004).

More recently, large CH^+ abundances have also been inferred from the first detection of the $^{13}CH^+(J{=}1\text{-}0)$ line at $\nu = 830.1$ GHz by Falgarone, Phillips & pearson (2005) in absorption against a remote star forming region. Broad and weak HCO^+(1-0) lines, observed in emission in diffuse molecular gas trace HCO^+ abundances more than two orders of magnitude larger than those predicted by steady-state chemistry in that kind of medium (diffuse and $A_v \leq 1$) (Falgarone et al. 2006).

H_2 also appears to be more excited in diffuse molecular gas than predicted by PDR models. This excess of excitation is not due to the release of energy due to H_2 formation (Lacour et al. 2005). The signature of myriads of small pockets of warm gas in the diffuse medium may have been detected in the lowest rotational transitions of H_2. In *ISO-SWS* observations of a long line of sight through the Galaxy, avoiding regions of massive star formation, the intensities of the S(1) and S(2) lines exceed, by almost an order of magnitude, those expected from modelling the PDR-type emission of that line of sight. The excitation of these transitions has to be collisional in gas hotter than PDR material irradiated by the ambient UV field (Falgarone et al. 2005). The observed H_2 emission was ascribed to a large number of MHD shocks (Flower & Pineau des Forêts 1998) or coherent small scale vortices (Joulain et al. 1998), two processes responsible for the bursts of dissipation of MHD turbulence. Only a few percents of warm H_2 on the line of sight (*i.e.* H_2 molecules in $J_u > 2$ levels) are required to reproduce the observed line intensities. The same fraction of warm H_2 in the total gas column is derived from far UV spectroscopy with *FUSE* in the direction of three nearby late B stars (Gry et al. 2002). Interestingly, observed CH^+ column densities in the Solar Neighborhood are correlated to those of excited H_2 (Lambert & Danks 1986) but are about 100 times above the PDR predictions.

These results suggest that the existence, within the cold neutral medium, of a small fraction of warm molecular gas, for which UV photons cannot be the sole heating source, is ubiquitous, and presumably traces the intermittent dissipation of non-thermal (turbulent) energy in the cold gas.

3 Dissipative structures in the turbulent ISM

Interstellar turbulence in the CNM being magnetized, with neutrals only partially coupled to the magnetic fields, one of the dominant dissipation mechanism is due to ion–neutral friction, either in MHD shocks (Flower

& Pineau des Forêts, 1998), Alfvén waves (Zweibel & Josafatsson 1983), or coherent magnetized vortices (Joulain et al. 1998). Reconnection in thin current layers promoted by ion–neutral drift may also operate (Zweibel & Brandenburg, 1997; Heitsch & Zweibel, 2003). In all cases, whatever the process (or coupled processes) responsible for it, this dissipation is intermittent in space and time. Observed scaling laws between velocity v_l and scale l in interstellar turbulence provide an estimate of the *average* kinetic energy transfer rate in the diffuse medium (average density $\overline{n} = 30\ \mathrm{cm}^{-3}$ and mean mass per particle $\mu = 1.33$ uma) of $\overline{n}\mu v_l^3/l \approx 2 \times 10^{-25}\ \mathrm{erg\,cm^{-3}s^{-1}}$ (Falgarone, Hily-Blant & Levrier, 2004). In more practical units, this corresponds to a specific luminosity $\approx 10^{-3} L_\odot/M_\odot$ to be compared to that of the UV photons. These values show that in order to produce significant heating of the gas and generate observable signatures turbulence has to be dissipated in less than one thousandth of the whole "volume" pervaded by turbulence.

3.1 How to locate dissipative structures in diffuse molecular gas?

Because turbulence most intense dissipation affects only a tiny fraction of the gas, its signatures are difficult to detect individually. Statistical methods, inspired from laboratory experiments, have been developed. They rely on a fundamental property of turbulence: all the quantities involving velocity differences between two points (shear, vorticity, velocity increments and dissipation) have non-Gaussian probability distributions (PDF) and the departure from a Gaussian PDF increases as the lag decreases.

The difficulties specific to astrophysical measurements are twofold: (1) the line-of-sight projection of the velocity and plane-of-sky projection of the displacement, (2) the large size of the sample and its homogeneity required to build reliable statistics, down to probabilities $\approx 10^{-4}$. A method based on the statistics of line centroid velocity increments (CVIs), first proposed by Lis et al. (1996), allows to locate the positions that build up the non-Gaussian tails of the PDFs (Pety & Falgarone 2003). Applied in large ^{12}CO(1-0) maps of diffuse molecular clouds, this method shows that the positions populating to the non-Gaussian tails of PDFs at small lags are not randomly distributed: they form filamentary structures of thickness ranging from 0.03 pc, down to less than 0.01 pc for those unresolved (Hily-Blant 2004, Hily-Blant et al. in prep.). They are a novel kind of small scale structures in interstellar clouds because they do not coincide with any small scale density or column density enhancement, but with gas optically thin in ^{12}CO(1-0), warmer and more diluted than the bulk of the gas (Hily-Blant & Falgarone 2006). This is the first time that such an association between large velocity shears (or CVIs) and gas warmer than its environment is suggested, in agreement with the fact that viscous dissipation, and therefore heating, scales as the square of the velocity shear.

Observations with the Plateau de Bure interferometer have resolved one of these regions of large CVIs into two almost parallel elongated structures, separated by 3.5 km s^{-1} (Falgarone et al. in prep.). If they are as close to each other in space as they appear in projection (separated by less than 10" or 1500 AU) the inferred shear is as large as $\sim$ 500 km s^{-1} pc^{-1}, still larger than the value $\sim$ 40 km s^{-1} pc^{-1} observed over 0.05 pc in high latitude clouds by Sakamoto (2002). The associated timescale is only $\approx 2 \times 10^3$ yr. Velocity shears, occasionally orders of magnitude larger than the average value observed in molecular clouds $\sim$ 1 km s^{-1} pc^{-1}, seem to exist at small scales in the diffuse parts of molecular clouds. Note that the above value of the velocity shear is even larger than predicted on the basis of the scaling laws $\nabla v \propto l^{-2/3}$. Signatures of intermittent dissipation of turbulence (thermal, chemical, dynamical) are thus expected to be most prominent at small scales.

3.2 Non equilibrium chemistry in the CNM

We give here the outline of a model of dissipative structures, intended to capture the essence of what could be an alternative to magneto-hydrodynamic (MHD) shocks in the absence of obvious post-shock compressed layer. Following Moffatt, Kida & Ohkitani (1994), the regions of intermittent dissipation have been modeled by Burgers vortices threaded by helical magnetic fields (Joulain et al. 1998). The vortex is fed by large scale motions, so its lifetime is of the order of the turnover time of the large scales, ten times (or more) its own period, P. In the model illustrated in Fig. 1, the period of the vortex is $P = 600$ yr, its lifetime $\approx 10^4$ yr, and the minimum time to build up the molecular abundances specific of the warm chemistry is $t_{warm} \approx 200$ yr. The large differences between these timescales justify that we compute the time-dependent chemical evolution of the gas spiralling in a steady-state magnetic and dynamical configuration of the vortex. Its characteristics are not free parameters but imposed by the ambient turbulence: its radius sets the local viscous dissipation rate (Fig. 1), its finite length

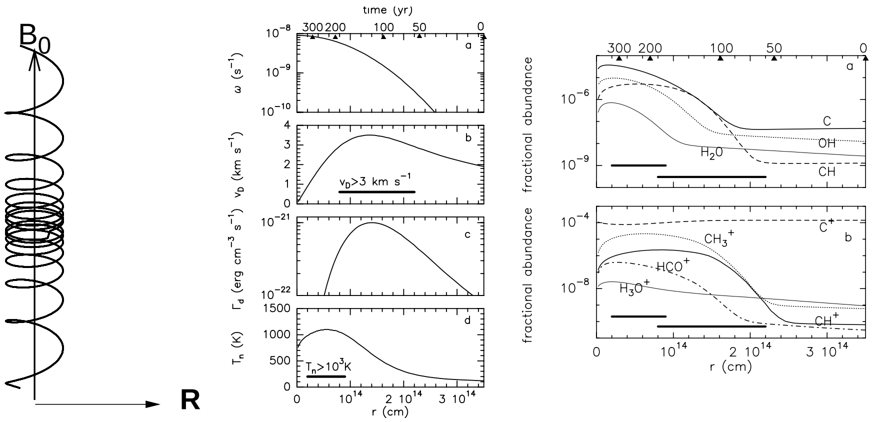

Fig. 1. *Left:* Steady-state configuration of **B** imposed by boundary conditions and vortex motion in the neutrals, *Middle:* from top to bottom, the vorticity, the ion-neutral drift velocity (or the azimuthal velocity of the neutrals), the viscous heating rate and the resulting temperature, all drawn as a function of the distance to the vortex axis. The time (arbitrary origin) is shown on the upper scale. The *active* layers of the vortex are underlined by the thick segments. *Right:* Run of the fractional abundance of a subset of molecules along their spiral motion towards the axis of the vortex. From Joulain et al. 1998.

is at the origin of the helical configuration of the magnetic fields in weakly ionized gas. Two heating sources dominate those due to UV photons: viscous shear and friction between the neutrals and ions tightly coupled to the steady helical fields. The Lagrangian time-dependent chemical evolution of a cell spiralling inwards in the vortex is computed. It involves 41 species and 278 reactions. As shown in Fig. 1, it reacts swiftly to the sharp increase of gas temperature generated by turbulence dissipation.

The gas is heated and enriched chemically during at least 200 yr while it crosses the layers of largest velocity shear and largest ion-neutral drift, the *active* layers of the vortex (underlined in Fig. 1). As it enters the central regions of the vortex where the temperature drops due to the decrease of dissipation, the gas starts cooling down, relaxes chemically and condenses self-consistently with chemistry. Its radial and orthoradial velocities there have vanished and the gas escapes along the vortex axis. Eventually, the vortex blows-up, after $\approx 10^4$ yr. The thermal and chemical relaxation of the gas once it has escaped the *active* layers of the vortex has been computed in Falgarone et al. 2006, assuming an isobaric evolution. It is remarkable that the signatures of the warm chemistry are kept by the gas for more than 10^3 years after the gas has escaped the active layers. Moreover, during the relaxation phase, the computed OH/HCO^+ and OH/H_2O abundance ratios are close to those observed (Neufeld et al. 2002, Liszt & Lucas 1996).

It is also encouraging that the relaxation tracks for HCO^+ are consistent with the abundances, density and temperatures inferred from the observations mentioned in Section 2. Moreover, the proposition that the products of "warm" chemistry build up at the expense of turbulent kinetic energy is supported by the observed anticorrelation of the column density of HCO^+ and the line width (Falgarone et al. 2006).

4 The bright and steep road ahead

The picture emerging from the recent observations reported above is that of a cold diffuse medium structured down to AU scales by the dissipation of turbulence, heterogeneous in temperature and density beyond the traditional picture of "clumps", evolving chemically over timescales of a few 100 yr, and out of thermal and chemical equilibrium. In the scenario outlined above, traces of warm gas enriched chemically coexist, even in a small telescope beam, with larger amounts of cold gas, already relaxing. This illustrates the difficulties met at interpreting molecular line emission, when, in reality, time averages are observed. A powerful information is borne by the velocity field, and this is the strength of heterodyne observations. The observations of Herschel/HIFI will provide most sensitive diagnostics of "warm" chemistry in the CNM and ALMA should be able to map the pronounced kinematic and chemical signatures of turbulence dissipation at the AU scale in nearby clouds.

References

Black J.H. & Dalgarno A. 1977 ApJS 34 405

Crane P., Lambert D.L. & Sheffer Y. 1995 ApJS 99 107

Elitzur M. & Watson W.D. 1980 ApJ 236 172

Falgarone, E., Hily-Blant, P. and Levrier, F., 2004, ApSS 292,89

Falgarone E., Phillips T.G. & Pearson J.C. 2005 ApJL 634 L49

Falgarone E., Pineau des Forêts G., Hily-Blant P., Schilke P., 2006, A&A in press

Falgarone E., Verstraete L., Pineau des Forêts G., Hily-Blant P., 2005 A&A, 433 997

Flower D. & Pineau des Forêts G. 1998 MNRAS 297 1182

Gredel R. 1997 A&A 320 929

Gry, C., Boulanger, F. Nehmé, C., Pineau des Forêts, G., Habart, E. and Falgarone, E., 2002 A&A 391, 675

Heitsch F. & Zweibel E. 2003 ApJ 590 291

Hily-Blant P. & Falgarone E. 2006 A&A accepted

Hily-Blant, P., 2004, PhD Université Paris-Sud

Joulain K., Falgarone E., Pineau des Forêts G., Flower D. 1998 A&A 340 241

Lacour S., Ziskin V., Hébrard G., et al. 2005 ApJ 627 251

Lambert D.L. & Danks A.C. 1986 ApJ 303 401

Lis D., Pety J., Phillips T.G. & Falgarone E. 1996 ApJ 463 623

Liszt H.S. & Lucas R. 1996 A&A 307 237

Lucas R. & Liszt H.S. 2000 A&A 355 333

McKee C.M. & Ostriker J. 1977 ApJ 236 172

Moffatt H.K., Kida S. & Ohkitani K. 1994 JFM 259, 241

Neufeld D.A., Kaufman M.J., Goldsmith P.F., Hollenbach D.J. and Plume R. , 2002, ApJ 580 278

Penzias, A.A., Solomon, P.M., Jefferts, K.B. & Wilson R.W., 1972 ApJL 174 L43

Pety, J. & Falgarone E., 2003 A&A 412 417

Plume R., Kaufman M.J., Neufeld D.A. et al., 2004 ApJ 605 247

Sakamoto S., 2002 ApJ 565 1050

Scalo J. & Elmegreen B.G. 2004 ARAA 42 275

Watson W.D. 1974 ApJ 189 221

Zweibel E.G. & Josafatsson K. 1983 ApJ 270 511

Zweibel E.G. & Brandenburg A. 1997 ApJ 478 563