THERMAL PROCESSES IN MOLECULAR GAS

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ABSTRACT. The dynamics of the cold atomic and molecular gas, on which we focus here, is strongly affected by non equilibrium heating and cooling processes. We give two different examples, in which the breaking of the thermal balance is due respectively to variations of the incident ultraviolet radiation flux, and non equilibrium abundances of H_2 molecules in molecular clouds envelopes. Fluctuations of the ultraviolet radiation flux in clumpy molecular cloud envelopes result in the formation or the destruction of dense regions. Large density contrasts, greater than one order of magnitude, are easily achieved in cloud regions of moderate visual extinction. Condensation or expansion develop on quite short time scales, of the order of a few tenth of million year, and induce collective motions which can feed turbulence.

Another example of the importance of out of equilibrium thermochemical processes is furnished by the study of the $H - H_2$ transition layers in molecular clouds envelopes. They turn out to be unstable against convection-like motions, driven by the energy released by H_2 photodestruction. The gas velocities involved in these motions are, again, typical of the observed turbulent velocity in clouds envelopes.

Keywords: Interstellar medium: clouds - Interstellar medium: kinematics and dynamics of - Interstellar medium: thermal processes.

1. Introduction

Roughly speaking, the interstellar gas has the unusual property to get cooler with increasing density. However, this is only true if one assumes *thermal balance* between the various heating and cooling processes. Large departures from thermal equilibrium are easily achieved in (hydro)dynamical processes, which can result from an instability - such as thermal instability - or can be triggered from the environment. Since the work of Field, Goldsmith and Habing (1969), thermal instability has been extensively studied, in particular in the context of HI cloud formation and cooling flows. Recently, Balbus (1986,

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1988) and Balbus and Soker (1989) have established a close connection between thermal instability and convection. Hattori and Habe (1990) have performed two–dimensional hydrodynamical calculations of thermal instability in cooling flows.

The heating or cooling times in the envelopes of molecular clouds are of the order of a few tenth of million years. By no means the thermodynamic evolution of the gas can be properly mimicked by a definite polytropic transformation, since the polytropic exponent Γ (such that locally $P \propto \rho^\Gamma$) depends explicitely on the rate of variation $\omega = 1/\rho \, d\rho/dt$ of the density. This is due to the fact that the heating and cooling terms do have finite characteristic times which have to be compared to the hydrodynamical time scale ω. Accordingly, reasonable approximations to the heating and cooling term, when coupled to hydrodynamics, reveal a new class of phenomena closely related to clump formation and turbulence in molecular cloud envelopes.

The thermal balance of the gas can be affected in three different ways. First, variations of the density influence markedly the collisional cooling terms (per atomic hydrogen nucleus), since they are proportional to the density. Second, variations of the incident ultraviolet radiation flux alter the dust grain photoelectric heating rate, including or not heating by PAHs, which are dominant in regions with visual extinction $A_v \leq 3\ mag$. Large ultraviolet intensity fluctuations are suggested by the analysis of the tranfer in clumpy media (Boissé 1990). Finally, various species which play an important role in thermal processes, such as CO, C^+ or H_2, can be brought far from their chemical equilibrium abundances by the hydrodynamical evolution of the gas. In each case, the actual thermal pressure of the gas can be very different from the estimates based on the assumption of thermal balance. The resulting non uniform pressure or temperature variations may dominate the dynamics of the interstellar gas.

In the followings, we illustrate these points by two examples, in which we analyze some consequences of local variations of the UV incident flux, due to density inhomogeneity, and the effect of turbulence in the transition region of a molecular cloud where the gas turns from atomic (HI) to molecular (H_2). In the first case, the extinction variations result essentially in the condensation of the shielded regions. In the second case, a strong instability is shown up, which is closely akin to convection.

2. The gas response to fluctuations of the UV radiation field

Many clumps in clouds envelopes have masses far below the Jeans mass, and exhibit clear cut edges, hardly reconciliable with a strict gravitational origin. Up to extinctions $A_v \sim 3\ mag$, the interstellar ultraviolet radiation flux regulates the physical state of large amounts of molecular gas. Thus, it should play an important role in the formation of such clumps, through the ionization of carbon atoms and dust grain photoelectric heating. Very small particles or PAHs may be a major source of heating of the low density gas (d'Hendecourt and Léger 1987, Lepp and Dalgarno 1988, Puget and Léger 1989). However, charge effects both on the dust grain or PAH photoelectric heating rates push the threshold of thermal instability down to a density lower than $n_H \sim 1\ cm^{-3}$.

Even in the absence of thermal instability, spatial fluctuations of the local UV intensity generate a non uniform thermal balance and substantial density variations are achieved when the gas tends to recover local thermal equilibrium. This dynamical process sets matter in motion, for at least two reasons: condensation (expansion) flows are expected in cooling (heating) regions, and the formation of density inhomogeneities upsets the local hydrostatic equilibrium, giving rise to bulk motions driven by the Archimedes force.

The description of the actual dynamics requires a careful treatment of the hydrodynamical interactions between regions with different thermal evolutions (see Sect.3). However, useful informations can be easily obtained if one assumes that the perturbed regions roughly remain in pressure equilibrium with the unperturbed surroundings.

We first present the *isobaric* gas response to an external attenuation of the UV field, which, due to the strong decrease of the dust grains photoelectric heating rate, leads to the condensation of the cooling gas. The adopted unpertubed UV intensity, at zero visual extinction, is (Mathis *et al.* 1983): $\phi_0 = 2.5\ 10^{-8} - 4.6\ 10^{-8}$ $photon\ cm^{-2}\ s^{-1}\ Hz^{-1}$ at 1000 and 1101 Å. Indirectly, the abundances of the major cooling and heating agents (C^+, CI, OI, CO, H_2) are altered during the evolution. The time dependent abundances are calculated using a realistic chemical network (Pineau des Forêts *et al.* 1988) and the method described by Heck *et al.* (1990).

Regarding H_2 photodestruction, self-shielding is treated following de Jong *et al.* (1980), with the rate:

$$R_D(H_2) \ = 4.\ 10^{-11}\beta(\tau_{H_2})exp(-2.5A_v) \quad s^{-1} \tag{1}$$

where A_v is the visual extinction, $\beta(\tau_{H_2})$ is the probability that UV photons penetrate in the considered region of a cloud with optical depth τ_{H_2}, related to the H_2 column density by (de Jong *et al.* 1980):

$$\tau_{H_2} = 1.2\ 10^6 \left(\frac{\mathcal{N}(H_2)}{10^{20}\ cm^{-2}}\right)\left(\frac{\delta V_D}{1\ km\ s^{-1}}\right)^{-1} \tag{2}$$

where δV_D is the gas velocity dispersion. A difficulty arises in the evaluation of this latter expression, since the total shielding H_2 column density, $\mathcal{N}(H_2)$, is *a priori* unknown. It could be calculated self-consistently at each point of a cloud model, at the cost, however, of a loss of generality. We choose to estimate the value of the optical depth τ_{H_2} as a function of the visual extinction A_v, using the observed correlation between $\mathcal{N}(H_2)$ and the color excess E(B-V) (Savage *et al.* 1977), and assuming a constant color ratio R=A_v/E(B-V)=3.2. The resulting function $\tau_{H_2}(A_v)$ exhibits a sharp discontinuity of the H_2 self-shielding at the visual extinction $A_v^* = 0.25\ mag$.

The gas density evolution (at constant pressure P_0) which follows the extinction perturbation ΔA_v is described by the equation:

$$\frac{dn}{dt} = \frac{2}{5}\frac{n\mathcal{L}}{P_0} + \sum_i \left(\frac{dn_i}{dt}\right)_{ch} \tag{3}$$

where $\mathcal{L}$ is the net cooling rate per unit volume (cooling minus heating), n is the total number density of particles and the index "ch" denotes purely chemical transformations. The temperature T of the gas obeys the equation:

$$\frac{dT}{dt} = -\frac{2}{5}\frac{T\mathcal{L}}{P_0} - \frac{T}{n}\sum_i \left(\frac{dn_i}{dt}\right)_{ch} \tag{4}$$

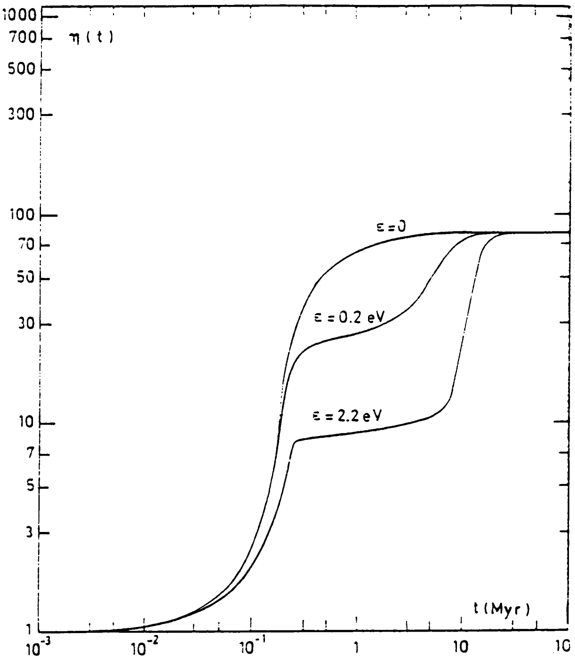

Figure 1: *Time dependent isobaric condensation in low density gas following an extinction variation $\Delta A_v = 1$ mag. Curves are labeled with three distinct values of the kinetic energy released per H_2 formation.*

The condensation factor $\eta(t) = n_H(t)/n_H(t=0)$ is presented in Fig.1 for the cloud envelope initial conditions $n_{H_0} = 20\ cm^{-3}$, $A_{v_0} = 0.25\ mag$. The visual extinction is decreased by two magnitudes. The condensation factors are calculated for three different values of the uncertain kinetic energy input due to H_2 formation on dust grains, $\epsilon(H_2)$ (Williams 1987). The condensation factor increases with larger incident UV flux. A typical value $\eta = 10$ is achieved in denser gas, $n_{H_0} = 100\ cm^{-3}$ with extinction $A_{v_0} = 0.5\ mag$ (de Boisanger and Chièze 1991).

The process discussed so forth is efficient in producing non gravitationally driven gas condensation by more than one order of magnitude. The amplitude of the condensation is higher in low density gas, in which it exceeds two orders of magnitude, than in $n_H \sim 100\ cm^{-3}$ gas for which density contrasts of about 10 are achieved. Quite naturally, a high UV intensity strengthens condensation. Furthermore, condensation factors are quite sensitive – through the heating rate – to the grain size, the photoelectric efficiency, the presence or not of PAHs, and – through the cooling rate – the depletion of carbon. The condensation growth time is always quite short: density enhancements by a factor of 10 are commonly achieved by $t \approx 0.1 - 0.2\ Myr$, which is about two orders of magnitude shorter than the free fall time. The linear size of the condensed regions depends only on the coverage of the perturbation.

3. Two dimensional hydrodynamical simulations

Hydrodynamical simulations, including the relevant heating and cooling terms, confirm the values of the condensation factors, and present further the advantage of a correct estimation of the *velocity field* induced by the extinction perturbation. As an example of such calculations, Fig. 2 represents the gas response to a (gaussian) perturbation of the extinction of 1 mag, moving with the velocity $v = 0.2\ kms^{-1}$. The gas is initially thermally balanced and in hydrostatic equilibrium with a density of 30 cm^{-3} at the free surface, and $10^6 cm^{-3}$ at the base of the structure, while the (unperturbed) extinction varies from 0.1 mag to about 100 mag. Lateral periodic conditions are assumed, together with a fixed boundary at the base, and a free surface maintained at constant pressure throughout the calculation.

The condensation lags slightly behind the position of the perturbation, and induces a convection–like velocity pattern with a maximum velocity $v_{max} = 0.7\ km\ s^{-1}$ after 1 Myr, which steadily increases with time up to 0.9 $km\ s^{-1}$ for $t \geq 3$ Myr. Downwards velocity in the condensed material are set up by the Archimedes force. Two rarefaction waves are naturally driven on both sides of the condensation, which result in gas heating and upwards motions.

The nature of this mechanism favors the growth of “elephant-trunk” shaped condensations, and can be a source for turbulence in cloud envelopes.

4. Instability of the $H - H_2$ transition layer

Molecular clouds are generally closely associated with large amounts of atomic hydrogen. Due to H_2 self–shielding, the transition to molecular hydrogen is very sharp, and occurs in a cloud at an extinction level of $Av \sim 0.25 - 0.5\ mag$. Loosely speaking, the gas located below this level is mostly molecular, while it is mostly atomic above. In other words, large amounts of H_2 molecules are present in the vicinity of a region where they can be quickly photodissociated.

This is not without sequel if one consider that cloud envelopes are turbulent. Since the gas velocity dispersion in cloud envelopes is at least of the order of $\sigma_v = 0.5\ km\ s^{-1}$, mixing should occur accross the transition layer. As a consequence, H_2 molecules advected in the essentially unshielded regions are rapidly destroyed, releasing an amount $\Delta\epsilon = 0.5\ eV$ of kinetic energy per photodestruction. This is a large extra heating term for still H_2-rich rising parcels of gas, which, in most cases, overçomes adiabatic cooling due to their expansion in the decreasing pressure gradient of the cloud envelope.

The problem is closely related to convection, at least in its simplest acceptation. Consider a gas bubble perturbed from its original position in the shielded region. We follow its motion in the $HI - H_2$ transition layer, that is the region where the UV optical depth τ_{H_2} varies abruptly, by calculating the thermal balance between the various cooling

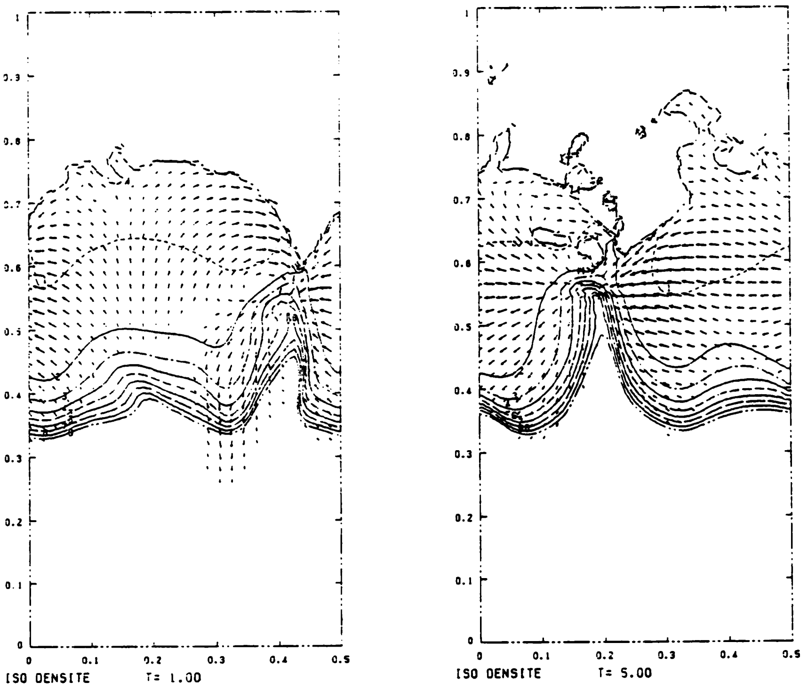

Figure 2: *Two dimensional simulation of a cloud envelope perturbed by an extinction variation* $\Delta A_v = 1$ *mag moving with a velocity of* 0.2 *km* s^{-1}. *Density contours are equally spaced from* 50 *to* 850 cm^{-3}. *Low lying dense and heavily obscured material is unaffected by the perturbation. The maximum gas velocity is* 0.72 *km* s^{-1} *after* 1 *Myr (left) and* 0.90 *km* s^{-1} *at* $t = 5$ *Myrs (right). Horizontal and vertical scales are in parsecs.*

and heating processes, including notably cooling due to the expansion of the bubble and heating due to H_2 photodissociation. As in the standard analysis of convection, it is assumed that the rising gas parcell maintains pressure equilibrium with its unperturbed surroundings. If the temperature in the rising bubble turns out to be greater than the ambient temperature, the Archimedes buoyant force will reinforce its motion.

The result is that, despite the fact that the outward entropy gradient in a molecular cloud envelope is markedly positive – which means convective stability according to the classical ***adiabatic*** Schwarzschild criterion – the energy deposition by H_2 photodissociation is by far sufficient to induce large buoyant forces. By contrast with convection as generally treated in the context of stellar models, the motion of moving fluid elements in a molecular cloud are strongly non adiabatic, due to the presence of many heating and cooling processes, always unbalanced in a time dependent thermodynamical evolution. Calculations show that the Archimedes acceleration is in most cases greater than the gravitational acceleration by more than a factor of 10. Neglecting viscosity (and hydrodynamics) it would result in bubbles rising soon at supersonic velocities. Thus, if some amount of turbulence is required to trigger the instability, it is likely to be amplified in these regions of cloud envelopes.

5. Conclusions

The examples we have presented stress the role of the heating and cooling processes both on non gravitational condensation of molecular gas and the generation of a complex velocity field, comparable in magnitude to the observed turbulent velocities. By itself, the UV process does not produce very high density clumps, but since the Jeans mass varies as η^{-2} during an isobaric condensation, local decrease of the Jeans mass by two or three orders of magnitude are expected to occur in regions shielded from UV exposure by preexisting clumps. The condensation time scales are short, of the order of a few tenth of million years. Since the driving perturbations are not stationary, this means that molecular gas may experience large density and extinction variations with such short turn over time scales. From a complementary point of view, this points to non–equilibrium molecular chemistry. It should be noticed that calculations of chemical abundances taking into account short time scale mixing and density variations are effective in producing much larger amounts of complex molecules, together with high C/CO ratios, than equilibrium calculations (Chièze and Pineau des Forêts 1989, Chièze *et al.* 1991). Finally, thermal processes are able to induce large gas velocities, and thus should be considered as a natural driving term for cloud turbulence.

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