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CHEMISTRY AND DYNAMICS: A POST-PROCESSING TOOL TOWARDS A REAL COUPLING

V. Valdivia[1], B. Godard[2], P. Hennebelle[1], M. Gerin[2] and P. Lesaffre[2]

Abstract. Chemistry plays a key role in the comparison between observations and theoretical predictions, but its treatment in numerical simulations is a real challenge. In particular the full treatment of the chemistry requires to solve simultaneously hundreds to thousands of reactions, constraining the time-steps to be as small as the smallest one. Fortunately, several species reach the chemical equilibrium much faster than others, and careful choices allow to describe the chemical state in a simpler manner. Here we present a hybrid approach to treat the chemistry of the interstellar medium.

Keywords: Methods: numerical, ISM: clouds, abundances, Astrochemistry

1 Introduction

Chemistry is an essential component in the modelling of molecular clouds, but its complex description, which is coupled to the dynamics of the gas, makes it a commonly neglected issue.

Chemistry plays a key role in determining the thermal state of the gas. While the heating is ensured by the photoelectric heating (Bakes & Tielens 1994) on grains, in the case of molecular clouds, the cooling is realised by the line emission from atoms and molecules. Emission lines, and thus the ability to cool the gas, strongly depend on the abundance of the emitting atom or molecule, and thus on the chemical composition of the gas. On the other hand, the chemical structure of the gas is determined by the dynamics and the physical structure of the cloud. As different chemical tracers are sensitive to different physical conditions, the observed abundances not only allow to probe the medium, but also allow to link models to observations.

Even though the chemical state of the gas is crucial to predict its evolution, most of numerical simulations avoid the explicit treatment of the chemistry. Instead, heating and cooling functions are used to describe the thermal state of the gas. The advantage of using these functions is that they allow to produce realistic structures, being even able to reproduce the multiphase structure of the interstellar medium (ISM) (Audit & Hennebelle 2005; Valdivia & Hennebelle 2014; Valdivia et al. 2016c). These cooling functions can include several processes, such as the cooling by fine structure lines of CII, OI, and CI, cooling by H through the Lyman α emission, and the cooling due to electron recombination onto positively charged grains. These are usually subgrid models, which are functions of the local gas parameters. Furthermore, turbulence and magnetic fields not only controls the dynamics and the physical structure of the gas, but also influences the transport of atoms and molecules within the cloud.

In order to compare with available observations and make predictions, synthetic observables, such as synthetic spectra or synthetic maps, are needed. A simple approach consists in post-processing numerical simulations to obtain the expected abundances of atoms and molecules. These approaches can be as simple as applying a density threshold to estimate the molecular fraction of hydrogen (Heiner et al. 2015), or as sophisticated as the calculation of a full equilibrium using photon dominated regions (PDR) codes, for example (Levrier et al. 2012). The main advantage of this kind of approach is that exhaustive chemical networks (that depend on the local physical conditions of the gas), along with radiative transfer strategies, can be used. But this approach is not flawless. The main problem related to this approach is the fact that the chemistry does not evolve with

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[1] Laboratoire AIM, CEA/DSM-CNRS, Université Paris Diderot, IRFU/SAp, 91191 Gif-sur-Yvette, France
[2] LERMA (UMR CNRS 8112), Ecole Normale Supérieure, 75231 Paris Cedex, France

the gas, and the abundances miss some dynamical effects, or the underlying dynamics is imposed, as in the turbulent dissipation region (TDR) code (Joulain et al. 1998; Godard et al. 2009, 2014).

It is only very recently that the computational ressources have permitted to simulate 3-dimensional structures including explicit treatments for the chemistry. In recent years several efforts to couple the chemical evolution to the dynamical evolution of the gas have been attempted, either by including dedicated chemical networks into widely used codes (Glover & Mac Low 2007a,b; Glover et al. 2010; Koyama & Inutsuka 2000; Clark et al. 2012; Dobbs et al. 2008; Ziegler 2016), or either by developing general chemistry packages that can be plugged to them (Grassi et al. 2014). Time dependent chemistry has the advantage that the chemical abundances evolve with the gas, where they are not only formed and destroyed, but they can also be advected or diffused during the simulation, and thus capture the effect of the dynamics. But this kind of simulations is extremely prohibitive. The computation of the abundances can reveal itself extremely expensive. Computation times can be as high as several hundreds of times the usual computation time even for a modest chemical network. To deal with this problem most simulations use reduced chemical networks (Glover & Mac Low 2007a,b; Hocuk & Cazaux 2015; Hocuk et al. 2016), and uses further approximations to deal with complicated calculations, such as the computation of column densities and shielding parameters (Richings & Schaye 2016).

So the question that arises is how to take into account the dynamical effects on the chemical abundances, including good estimates of shielding parameters, and without excessively increasing the computation time? Even though the questions seems to have no answer, it is possible to address it by making clever choices.

Here we describe a hybrid strategy that can help to deal with this problem in numerical simulations in the context of the evolution of molecular clouds.

2 Hybrid strategy

2.1 General idea

Chemical species have very different evolution times. Species with long evolution times are most likely influenced by the gas motions, and consequently can be found out-of-equilibrium. On the other hand, species with short evolution times quickly react to variations in their environment, and are prone to be at equilibrium and to follow the evolution of other dominant species. This behaviour allows us to propose a strategy to treat the chemical evolution of molecular clouds minimising the calculation time.

The first step is to identify the species with the longuest evolution times. These species need to be calculated on-the-fly, and ideally including good, but fast estimates for the parameters such as the shielding. The second step is to post-process the simulation using a chemical network, where the abundances of the species dynamically calculated in the simulation can be fixed. The rest of the species in the chemical network is calculated at equilibrium using the physical conditions of the cloud.

2.2 On-the-fly treatment: H_2 chemistry

In the context of the interstellar medium a key molecule is the molecular hydrogen (H_2). This molecule has a very long evolution time on the order of $t \sim \frac{10^9}{n\ [\mathrm{cm}^{-3}]}$ yr (Hollenbach & Salpeter 1971), where n is the number density of the gas. This molecule is of crucial interest because it precedes the formation of other molecules. The evolution of its abundance is well described by

$$\frac{\partial n_{\mathrm{H}_2}}{\partial t} + \nabla \cdot (n_{\mathrm{H}_2} \mathbf{v}) = k_1 n (n - 2n_{\mathrm{H}_2}) - k_2 n_{\mathrm{H}_2}, \tag{2.1}$$

where n is the total density of the gas, n_{H_2} is the number density of H_2, $\mathbf{v}$ is the velocity field, k_1 is the formation rate on grains, and k_2 is the photodissociation rate by ultraviolet (UV) photons. Equation 2.1 includes the evolution of the density of H_2 due to the formation and destruction processes, as well as an advection term. It is able to reproduce the evolution of H_2 without needing a costly chemical network. In a previous work (Valdivia et al. 2016c) we implemented the evolution of H_2 in the RAMSES code (Teyssier 2002), using our tree-based method (Valdivia & Hennebelle 2014) to estimate column densities, as well as the visual extrinction A_V, and the H_2 shielding parameter $f_{\mathrm{sh,H}_2} = \exp(-\tau) \times f_{\mathrm{shield}}(\mathcal{N}_{\mathrm{H}_2})$, due to the combined action of the dust and the selfshielding (Draine & Bertoldi 1996) by H_2. In this expression τ is the optical depth, and $\mathcal{N}_{\mathrm{H}_2}$ is the H_2 column density. Numerical simulations show an important fraction of H_2 out of equilibrium that can play an important role in the chemical evolution of the cloud (Valdivia et al. 2016c).

2.3 *Post-treatment: the chemical solver*

The rest of the abundances in the chemical network (described later) is calculated by post-processing using a chemical solver. The chemical solver used in this work is a modified version of the solver used by the Meudon PDR code (Le Petit et al. 2006), that allows us to fix the abundance of H_2. It solves a coupled system of equations using a Newton-Raphson scheme to find the equilibrium for the chemistry. The equilibrium is defined by the following set of equations:

$$\begin{aligned} \frac{dn(\mathrm{X}_i)}{dt} &= \sum_j^{N_\mathcal{R}} \left(\prod_k n(\mathrm{R}_{j,k})\right) \kappa_j\; s_j(\mathrm{X}_i) = 0, && \forall i \in [1:N_X] \\ \sum_j^{N_X} n(\mathrm{X}_j)\; m(\mathrm{A}_i, \mathrm{X}_j) &= n_{\mathrm{A}_i} && \forall i \in [1:N_A] \\ \sum_j^{N_X} n(\mathrm{X}_j)\; c(\mathrm{X}_j) &= 0, \end{aligned} \tag{2.2}$$

where $n(\mathrm{X}_i)$ is the number density of the $i-th$ species, n_A is the number density of atom A, $N_\mathcal{R}$ is the number of reactions, $\mathrm{R}_{j,k}$ stands for the reactants, κ_j is the reaction rate of reaction j, $s_j(\mathrm{X})$ the stoichiometric coefficient of X in reaction j, $m(\mathrm{A},\mathrm{X})$ the multiplicity of atom A in species X, and $c(\mathrm{X})$ the charge of X.

The main input parameters are the total gas density n, the kinetic temperature T_k, the external UV radiation field χ, the visual extinction A_V, the cosmic ray ionisation rate ζ_{H_2}, and optionally the H_2 number density $n(\mathrm{H}_2)$, the shielding parameters $f_{\mathrm{sh,H}_2}$, $f_{\mathrm{sh,CO}}$, and the ion-neutral drift velocity v_d.

When the H_2 abundance is fixed the system of equations is overdetermined and at least one other species must be fixed to guarantee the conservation. We assume that atomic hydrogen is the only species out-of-equilibrium, along with H_2, due to its high abundance and because it is the main H-bearer besides H_2.

3 On the validity of the hybrid strategy

3.1 *Evolution time*

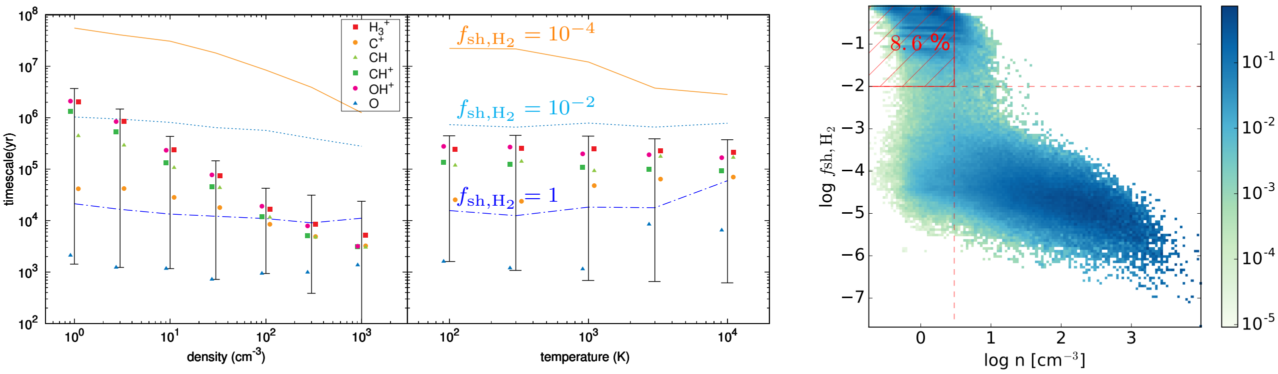

Fig. 1. Left: Chemical timescale averaged over random initial conditions. Lines correspond to the H_2 timescales computed for different shielding parameters: $f_{\mathrm{sh,H}_2} = 10^{-4}$ (solid), 10^{-2} (dotted), and 1 (dashed dotted). Vertical segments correspond to the interval of timescales for other molecules. Timescales for single species are shown for reference. **Right:** Gas mass distribution as a function of the density and the H_2 shielding parameter for a high-resolution simulation of a realistic molecular cloud.

Our approach is only valid if the evolution time of H_2 is longer than for the rest of the species. To test the validity of our approach in a range of different physical conditions we use a chemical network containing a total of 149 species and 2692 reactions, very similar to the one used by the Meudon PDR code. We computed the equilibrium timescales for all the species in the network under a wide range of physical conditions. Figure 1 shows the range of timescales for the species in the chemical network compared to the timescales for H_2. This figure helps us to constrain the conditions under which our approach is valid.

From the left-hand side panel of Fig. 1 we can identify a safe region, where the H_2 evolution timescale is always longer than (or comparable to) the evolution timescale of any other species in a wide range of physical conditions. As long as the gas number density is $n \gtrsim 3$ cm^{-3} or the H_2 shielding factor is $f_{\mathrm{sh,H_2}} \lesssim 10^{-2}$ the evolution time of H_2 will be long enough to guarantee that other species will have the time to reach their equilibrium.

To know whether this strategy is valid for numerical simulations of realistic molecular clouds it is essential to know the amount of matter that fullfils these conditions. The right-hand side panel of Fig. 1 shows the mass-weighted distribution of the gas in the high-resolution numerical simulation of Valdivia et al. (2016c, Appendix A). This figure shows that for a realistic molecular cloud these conditions are fulfilled in more than 91% of the mass of the gas.

3.2 *Convergence*

An issue of a different nature is the convergence of the solver. Fixing a species can prevent the existence of a solution for the equilibrium, or it can make it more difficult to reach. To determine under which conditions our approach is able to provide reliable results we performed a test covering a grid of 2.56 millions models in the 4D parameter space: density n, gas temperature T, H_2 fraction $f(H_2)$, and visual extinction A_V.

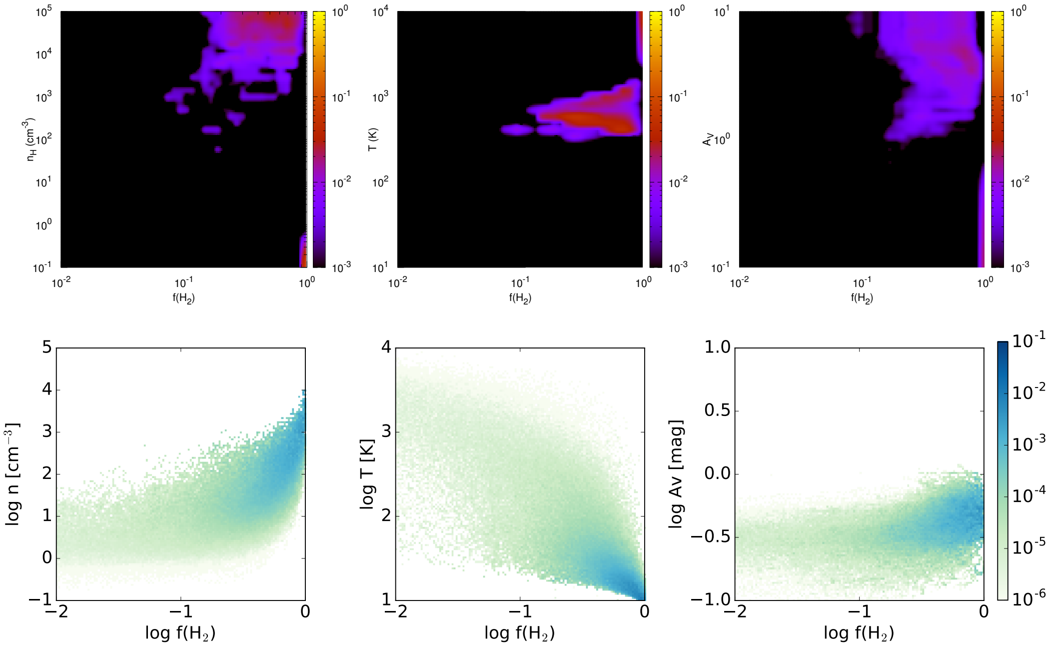

Fig. 2. Top: Fraction of convergence failures for 2.56×10^6 models in the 4D parameter space. **Bottom:** Mass fraction distribution in the simulation as a function of the same parameters.

The top panel of Fig. 2 shows the fraction of cases where the chemical solver fails to converge. This figure clearly shows two problematic regions in the parameter space. The most extended one corresponds to regions where the gas is dense ($n \gtrsim 10^3$ cm^{-3}), well shielded ($A_V \gtrsim 1$), with molecular fractions higher than 10^{-1}, and gas temperatures comprised between 300 K and few 10^3 K. These same models were tested without fixing the H_2 fraction showing similar results, which means that the failure is related to the algorithm and topology of the equation system. The second region, much more compact than the precedent one, corresponds to low density gas ($n \lesssim 1$ cm^{-3}), almost fully molecular ($f(H_2) \gtrsim 0.95$), illuminated ($A_V \lesssim 0.5$), and warm ($T \gtrsim 10^3$ K). In this case the chemical solver fails to converge due to the large abundance of H_2, which prevents the H conservation by other H-bearing species. The bottom panel shows the distribution of mass of the gas as a function of the same parameters. This figure shows that these cases are very unlikely to arise under realistic conditions for molecular clouds, and that our approach provides reliable results.

4 Conclusions

We showed that this approach is well adapted to treat numerical simulations of molecular clouds as long as the H_2 evolution time and the hydrodynamical time-step remain longer than the evolution time of the rest of the species. We assessed the convergence rate of the chemical solver for a wide variety of parameters. We showed the existence of two regions in the parameter space where the convergence fails.

We showed that a typical multiphase molecular cloud, submerged in the ISRF, displaying a wide variety of densities, temperatures, H_2 fractions, and shielding parameters, does not present gas in those problematic regions, and thus the solver is well adapted.

We conclude that our approach can be used to treat the chemistry of molecular clouds at a minimal cost compared to a time-dependent treatment of the chemistry. In a companion article we apply this hybrid approach to study the abundance of the methylidine cation (CH^+ molecule) in diffuse molecular clouds (Valdivia et al. 2016a,b).

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