

# TUTORIAL

# The Meudon PDR code

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# Introduction

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This document presents some exercises to learn to use the Meudon PDR code. They have been presented by Benjamin Godard at the french school about numerics, Astrosim, that took place in Lyon from the 26th June to the 7th July 2017.

The goal of the following exercises is to illustrate how the Meudon PDR model works. It thus includes the modification of the main input files, the visualisation and analysis of the results, and the exploration of the parameter space. This tutorial can be used with any version of the Meudon PDR code available on the ISM platform (<http://ism.obspm.fr>), including the current official release (PDR 1.5.2) and the simplified version (PDRLight).

The PDRLight version is faster to run than the standard PDR code. Note, however, that this version does not consider absorption of UV photons by the gas compounds such as, for instance, neutral carbon. PDRLight can be used for quick demos and is a valuable educational tool to understand the basics of code but using it for publications should only be done after a comparison of its results to those computed by the standard PDR code.



# Getting started

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## 2.1 Running a model of a standard diffuse cloud

Download the code (for instance PDRLight) from the website. Go in the `src` directory and configure the `Makefile`, in particular the compiler and the paths towards the `LAPACK` and `BLAS` libraries. Produce the `PDR` executable file using the `make` command. If you need help regarding the installation of the compilers and libraries, refer to the online documentation [here](https://ism.obspm.fr/files/PDRDocumentation/PDRDoc.pdf)<sup>1</sup>

Open the three main input file of the code to understand their structure:

- `data/pdr.in`
- `data/Chimie/ch1606_iso_Mathis.chi`
- `data/spectre.flag`

Tune the parameters in order to model a diffuse interstellar cloud with constant density,  $n_{\text{H}} = 100 \text{ cm}^{-3}$ , a dust / gas mass ratio of 0.01 and a fraction of PAH of 4.6 %. Set the size of the cloud  $A_{V,\text{max}}$  to 3 (expressed in magnitude of visual extinction) and the impinging radiation fields on both side to that of Mathis. To reduce the computational time, set the iteration number to 10 ; make sure however that all output files are produced (and not only the last two).

Go in the `src/` directory and run the code using the `../data/pdr.in` input file

```
./PDR ../data/pdr.in
```

To speed up the results analysis, a series of scripts is provided. Those must be moved:

```
scripts_extractor → AnalysisTools/Extractor/  
scripts_gnuplot   → out/  
scripts_UNIX      → out/
```

## 2.2 Extracting the results

During a run, the code builds a new directory (whose name is set in `pdr.in`) which contains all the results of the model. The main output files are written in HDF5 format and can be read with

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<sup>1</sup><https://ism.obspm.fr/files/PDRDocumentation/PDRDoc.pdf>

the `extractor.py` program using any computer. The iteration number of the output is indicated in the name of the file.

## Graphical user interface

Go in the `AnalysisTools/Extractor/` directory and run the program

```
python2.7 extractor.py
```

Open the *standard* HDF5 file (labeled `_s_`) corresponding to the first iteration.

Explore the tree structure and extract in a text file the distance from the edge of the cloud "`Distance`", the ionisation fraction "`Ionisation degree`", the gas temperature "`Tgas`" and the density of atomic carbon "`n(C)`". Open the file you created and understand its structure. Check that the cloud is symmetrical.

## Command line interface

The python program `extractor.py` can also be used with command lines (see the `README` file in the `Extractor` directory for more details). This option is very useful to systematically extract a large number of data computed by the code and stored in different HDF5 files.

To use `extractor.py` with command lines, the quantities to extract have to be written in a `.esf` file. The ascii file are then produced with the command

```
python2.7 extractor.py -f model.hdf5 -t script.esf -o result.txt -s " "
```

Go in the `AnalysisTools/Extractor/scripts_extractor/` directory and open all the `.esf` files. What kinds of quantities are listed ? Open the UNIX script `script_extract_all`, modify it if necessary, and run it in order to extract all the data listed in the `.esf` files for all the HDF5 files of the output directory.

## 2.3 Plotting and analyzing the results

## Analysis of the convergence

Go in the `out/model_name/` directory and open the file `model_name-10-phys.res`. Using the titles of the columns and a graphing utility software of your choosing, plot the evolution of the gas temperature as a function of the distance from the edge of the cloud (expressed in magnitude of visual extinction) obtained at the 10th iteration. If you wish, you can modify and use the script `scripts_gnuplot/temperature.gnu`.

Build similar figures for all the iterations and analyse the convergence of the code. What do you conclude for this example ? To automatize the production of figures, you can go in the `out/scripts_UNIX/` directory and modify and run the `temperature.sh` script.

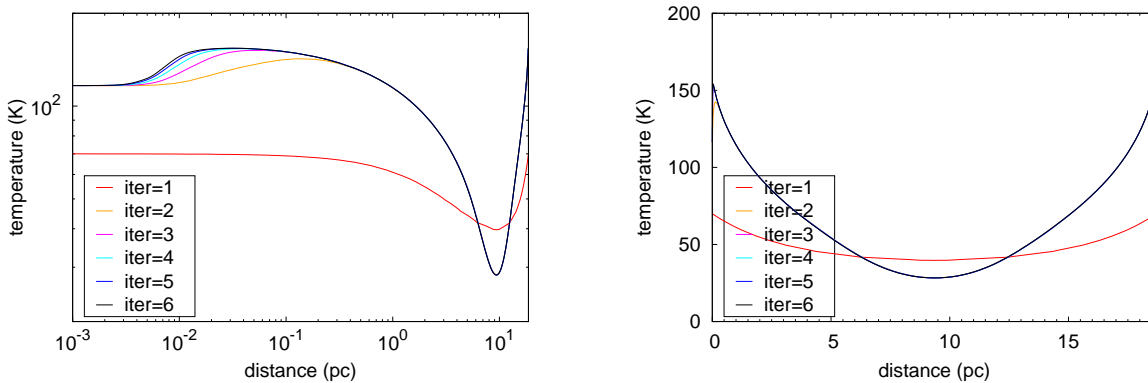


Figure 2.1: Gas temperature profile (in logarithmic or linear scale) of a typical diffuse molecular cloud with a size of 18 pc, a density 100 cm<sup>3</sup>, and illuminated on both sides by an isotropic radiation field of 1 (expressed in Mathis unit). The different curve correspond to different iteration numbers.

## Analysis of the temperature profile

We want to understand the temperature profile. To do that, plot the heating and cooling terms of the gas as function of the distance from the edge of the cloud. You can either look for these data in the `model_name-10-phys.res` file or use the gnuplot scripts, `scripts_gnuplot/heating.gnu` and `scripts_gnuplot/cooling.gnu`.

What happens for  $0.001 \leq A_V \leq 0.4$  ? Why ? To answer this last question, plot on three different figures the abundance profiles (1) of H and H<sub>2</sub>, (2) of C, C<sup>+</sup>, O and CO, and (3) of the electrons. These data are stored in `nom_modele-10-abon.res`. The figures can be produced with the gnuplot scripts, `transi-H-H2.gnu`, `transi-Cp-C-CO.gnu` and `electrons.gnu`.

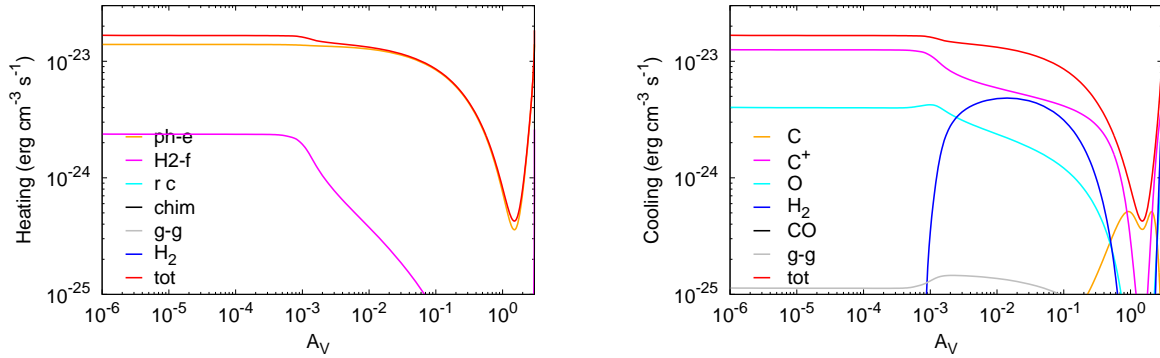


Figure 2.2: Heating and cooling terms of a typical diffuse molecular cloud with a size of 18 pc ( $A_{V,\max} = 3$ ), a density  $100 \text{ cm}^3$ , and illuminated on both sides by an isotropic radiation field of 1 (expressed in Mathis unit).

## Local analysis of the chemistry

We want to understand the peak of C abundance at  $A_V \sim 1.5$ . To do that, we need to analyse the chemical network at different points. Copy the *chemical* HDF5 file (labeled `_c_`) corresponding to the last iteration in the `AnalysisTools/ChemistryAnalyser/data/` directory.

Go in the `AnalysisTools/ChemistryAnalyser/server/` directory and open a local server  
`python2.7 server.py`

Go in the `AnalysisTools/ChemistryAnalyser/visualizer/` directory and run the chemistry analyser tool by opening the `index.html` file with a web browser. Open the *chemical* HDF5 file you just copied. What are the dominant reactions of formation and destruction of atomic and ionized carbon over the entire cloud ? To simplify, consider only the main processes which altogether contribute to more than 80 % of the total formation and destruction rates.

Plot  $n(\text{C}) + n(\text{C}^+)$  as function of  $A_V$ . Why is this sum constant ? With this result in mind and adopting the expressions of the chemical rates given below, find the system of equations that controls the abundances of C and  $\text{C}^+$ . Deduce analytical expressions for  $n(\text{C})$  and  $n(\text{C}^+)$  as functions of  $A_V$  and compare these expressions with the detailed calculation performed by the code. Conclude.

reaction	rate ( $\text{s}^{-1}$ )	indications
$\text{C} + \gamma \rightarrow \text{C}^+ + \text{e}^-$	$\sim 2.6 \times 10^{-10} \times G_0 \times \exp(-4 \times A_V)$	$G_0 = \text{Mathis field scaling (over } 4\pi \text{ sr)}$
$\text{C}^+ + \text{grains} \rightarrow \text{C} + \gamma$	$\sim 2.2 \times 10^{-08} \times n_{\text{PAH}}$	$n_{\text{PAH}} = 10^{-6} n_{\text{H}} = \text{PAH density (cm}^{-3}\text{)}$



# Going further - Exercice 1

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## 3.1 Model of a hot and dense PDR

Build a new input file to model the emission of a dense and hot PDR: set a constant density,  $n_{\text{H}} = 10^4$ ,  $A_{\text{V,max}} = 10$  and a strong UV radiation field (from the left side)  $G_0^- = 10^2$ . Don't forget to change the name of the output file in the input file to prevent overwriting your previous results. Last, modify the code to allow the analysis of line profiles: open the `PXDR_CONSTANTES.f90` file and set the `F_W_HDF5_ANA` parameter to 1.

Go to the `src/` directory, recompile the code and run this new model. Once the model has run, check its convergence and plot the temperature, heating, cooling, and ionization profiles, and the chemical transition of the dominant species. Compare the results with those obtained for a prototypical diffuse cloud. Explain the behavior of the  $\text{H}/\text{H}_2$  transition.

## 3.2 Emission line analysis

Extract the intensities of the 10 first rotational lines of CO and compare with the results obtained for a diffuse environment. Explaining the line intensities of chemical species is a complicated task. A line intensity results from the abundance of the species along the line of sight, the excitation conditions at each point (hence the temperature and the intensity of the radiation field at the transition wavelength), and opacity effects.

Choose a line among the CO ladder you just extracted. Plot the contribution of each point to the line emission, i.e. the `Contribution to intensities` variables stored in the *analysis* HDF5 file (labeled `_a_`) as function of the distance into the cloud. Compare this profile to the abundance profile of the upper level of the transition (variable `n(CO v=..., J=...)` in the *analysis* HDF5 file. Does the upper level peaks at the same position than the contribution ? What does it mean if it does not ?

Understand the profile of the upper level abundance. In such PDRs, CO is mostly excited through collisions with the main constituents of the gas. Plot the abundance profile of CO and the temperature of the gas as functions of  $A_{\text{V}}$ . Give an explanation for the observed profile.

### 3.3 Exploration of the parameter domain

The great advantage of 1D models is to allow the user to solve a large number of physical processes and their subsequent coupling within a reasonable amount of time: for the PDR code, the running time on a standard individual computer ranges from a few minutes (light version) up to several hours (complete version). This allows to explore the predictions of the model over a wide range of parameters, i.e. to apply the model to a variety of astrophysical objects: from the diffuse interstellar medium to the dense PDRs, in our Galaxy or even in extragalactic environments. This also allows to rapidly study the impact of a given parameter on the physical and chemical properties of interstellar matter.

Start from the previous model and choose a parameter to vary. Build five input files with different values of this parameter ranging over orders of magnitude and run the models. Check the convergence and compare the results with the previous one. Understand the differences using, if necessary the chemical and analysis HDF5 files.

### 3.4 Comparison with observations

Hot and dense PDRs are widespread environments in galaxies including the hot gas close to HII regions, diffuse and translucent clouds, protoplanetary disks, or the envelopes of dark clouds in star forming region complexes. In all these objects, PDRs line emission therefore act as valuable tracers, giving access to the state of the gas and dust, the energy balance, and the evolution of matter. Interpreting such observations, however, requires to explore the models over a wide parameter domain, understand and trust the predictions of physical quantities in this parameter space, and build a systematic and meaningful tool of comparison between observations and predictions.

To help the user exploring the PDR code, grids of precomputed models have been run and are stored on the ISM database [ISM database](https://ism.obspm.fr/)<sup>1</sup>. An online software is also provided to search for models that reproduce a set of observational constraints using sophisticated methods of data mining.

We consider here Spitzer/IRS observations of the rotational lines of  $H_2$  towards the reflexion nebula NGC 2023, a famous PDR illuminated by the hot B1.5 V star HD 37903. The analysis of these observations by Sheffer et al. (2011) lead to estimations of the column densities of the ground-state rotational levels which are given below.

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<sup>1</sup>[https://ism.obspm.fr/?page\\_id=403](https://ism.obspm.fr/?page_id=403)

J	energy (K)	column density ( $\text{cm}^{-2}$ )
2	509.850	$2 \times 10^{20}$
3	1015.153	$6 \times 10^{19}$
4	1681.678	$9 \times 10^{18}$
5	2503.870	$5 \times 10^{18}$
7	4586.377	$5 \times 10^{17}$

Assuming a 30% level uncertainty on the values given above, use the PDR database and the online software to find the isochoric model that reproduces the best the observational constraints. Download the model and study the physical structure of the cloud. Download and analyse other models in order to understand the maps provided by the Inverse Search Service.

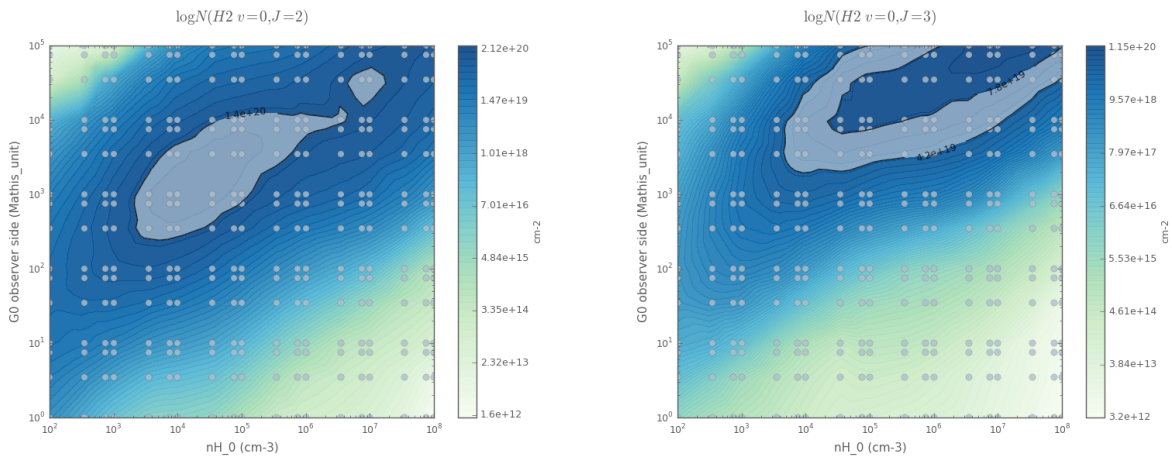


Figure 3.1: Column densities of the  $J = 2$  and  $J = 3$  levels of  $\text{H}_2$  as functions of the gas density and the strength of the radiation field for a cloud of size  $A_{V,\text{max}} = 1$ . The domain that reproduce the observations within their error bars are highlighted in grey.



# Going further - Exercice 2

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## 4.1 Model of dark environments

Build a new input file to model the rich chemistry of an interstellar cloud well shielded from the external UV radiation field: set a constant density,  $n_{\text{H}} = 10^4$ , and  $A_{V,\text{max}} = 30$ . Don't forget to change the name of the output file in the input file to prevent overwriting your previous results.

Go to the `src/` directory and run this new model. Once the model has run, check its convergence and plot the temperature, heating, cooling, and ionization profiles, and the chemical transition of the dominant species. Compare the results with those obtained for a prototypical diffuse cloud, in particular the  $\text{H}/\text{H}_2$  transition and the electronic fraction.

Find across the cloud the main carriers of carbon and oxygen, i.e. the species which store most of C and O elements in the cloud.

## 4.2 Exploration of the parameter domain

Start from the previous model and choose a parameter to vary. Build five input files with different values of this parameter ranging over orders of magnitude and run the models. Check the convergence and compare the results with the previous one. Understand the differences using, if necessary the chemical and analysis HDF5 files.