ISMServices

DOCUMENTATION

Chemistry Analyser (version 1.0.0)

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Presentation

The astrochemical models available on the ISM plateform are built to study the chemical state of interstellar clouds. Depending on the model, the chemical compositions of the solid phase and gas phase are computed either as functions of time by solving a system of coupled non-linear ODE (Paris-Durham shock code, TDR code) or at chemical equilibrium by finding the roots of a set of non-linear equations (Meudon PDR code). Since standard chemical networks contain several hundreds of species and thousands of reactions, these equations usually form a rather complex system. Analyzing and understanding the results of astrochemical models may therefore be difficult.

The Chemistry analyser tool is a software designed to open the HDF5 files produced by astrochemical models and perform detailed analysis of the computed chemical state as a function of the model main variable[1]. The analyser presents, in an interactive graphical user interface, schematic representations of the formation and destruction mechanisms of any species, and displays all the information necessary to analyse a given chemical state. In addition, the analyser allows to extract chemical rates in ASCII files or VO-Tables.

[1] This application is built on two open source javascript libraries available online: the dynamic, browser based visualization software `vis.js` (http://visjs.org) and the plotting library for jQuery `Flot` (http://www.flotcharts.org).

Overview

2.1 Installation and requirements

Several python packages are required to use the Chemistry Analyser. To facilitate its installation, an adequate python environment, `ismpy`, can be easily installed with the `install_ismpy.sh` script located in the Chemistry Analyser `scripts/` directory. The script will take care of installing all the required Python dependencies.

To **install the python environment**, type in a terminal from the Chemistry Analyser `scripts/` directory:

```
sh install_ismpy.sh
```

To **uninstall ismpy**, from the same `scripts/` directory, type:

```
sh install_ismpy.sh -d
```

To avoid any conflict with the system Python installation, all the material is installed in an independent *ismpy* Python installation[1]. The `ismpy` installation is located at `~/.ismpy/`.

Once installed this way, the `python` command to use ISM softwares as the Chemistry Analyser is located at: `~/.ismpy/bin/python3`

Alias for ismpy: It may be useful to define an alias for this python environment. To do so, add to the user's `~/.bashrc` or `~/.profile` file the line:

```
alias ismpy='~/.ismpy/bin/python3'
```

Besides python, the application requires a web browser.We currently recommend to use either `Google Chrome` or `Safari`. Performance issues have indeed been reported with both `Mozilla Firefox` and `Internet Explorer`.

[1] Actually ismpy is a virtual environment. So the python packages will be installed at the standard location in your computer. The /.ismpy/ directory contains only links with the proper PATHs.

2.2 Run the Chemistry Analyser

Once `ismpy` is installed, the Chemistry Analyser can be launched in two steps.

Run the Chemistry Analyser graphical interface:

1- In the Chemistry Analyser directory, type in a terminal: `sh chemanalyser.sh`

2- Open the `visualizer/index.html` with a web browser (ex: double click on it)

This will open the Chemistry Analyser in a window of your default web browser. Opening the index.html file you may wish to select a different web browser. We recommend to use either `Google Chrome` or `Safari`.

Analyse HDF5 output files

The PDR code and the shock code produce several HDF5 files. The Chemistry Analyser makes usage of the `_c.hdf5` files that contain the chemical network and the chemical reaction rates computed by the codes.

Output `_c.hdf5` files must be copied in the Chemistry Analyser `data` directory.

Important: Only _c.hdf5 files in the Chemistry Analyser data directory will be useable in the interface.

2.3 Organization

The Chemistry analyser is organized in two main menus, each designed to perform specific tasks

- `Control panel` contains inputs/outputs functions (e.g. export figures or files) and several options to set the general features of the graphics (e.g. threshold on the reaction rate).
- `Physical conditions` provides all the information necessary to analyze a given chemical state and allows to explore the chemistry as a function of the model main variable.

Control panel

3.1 Opening a HDF5 file

To open the result of a simulation, place the HDF5 file in the `data` directory and select the menu

```
Control panel > Data file > Model_c.hdf5
```

It produces a graphic which displays the main formation and destruction reactions of a species (by default H_2). These reactions are respectively shown on the left and right sides of the graph (Fig. 3.1). On both sides, reactions are organized from top to bottom in decreasing order of reaction rate.

The resulting graphic is fully interactive.

- Any element can be dragged to avoid ocasional crossings or to rearrange the global layout.
- Studying another species can be done by simply clicking on the species in the graphic.
- If the rate table is displayed, moving the mouse on any reaction in the graphic automatically highlights the corresponding reaction in the table.

3.2 Displaying the reaction rates

The values of the reaction rates, the rate constants, the abundances of the reactants, and the timescale of all the reactions displayed in the graphic can be obtained as a table with the option

```
Control panel > Reaction rates
```

3.3 Threshold on reaction rate

To avoid entanglements of reactions, the graphic only displays the reactions whose rates obey a given criterion. The nature of the criterion and its value can be changed with the options

```
Control panel > Threshold
```

Two methods are available so far.

- `minimum`: the graphic displays all reactions with rates above the threshold.

- `cumulated`: the graphic displays the successive dominant reactions which altogether contribute to a rate larger than the threshold.

If the `minimum` (resp. `cumulated`) threshold equals to 0 (resp. 100 %) all reaction rates are displayed in the table and the graph freezes to prevent entwining.

3.4 Extraction of data

The control panel finally allows the user to export data : the reaction scheme, the reaction rate table, the chemical network used, and the main formation and destruction reaction rates of the species `X` as functions of the model main variable. To perform this last task, use the option

```
Control panel > Export reaction rates
```

Two ascii files are then produced in the `save` directory containing respectively the destruction and formation rates of `X`: `destruction_X_Model.txt` and `formation_X_Model.txt`. Note that the operation can take a fair amount of time depending on the chosen species.

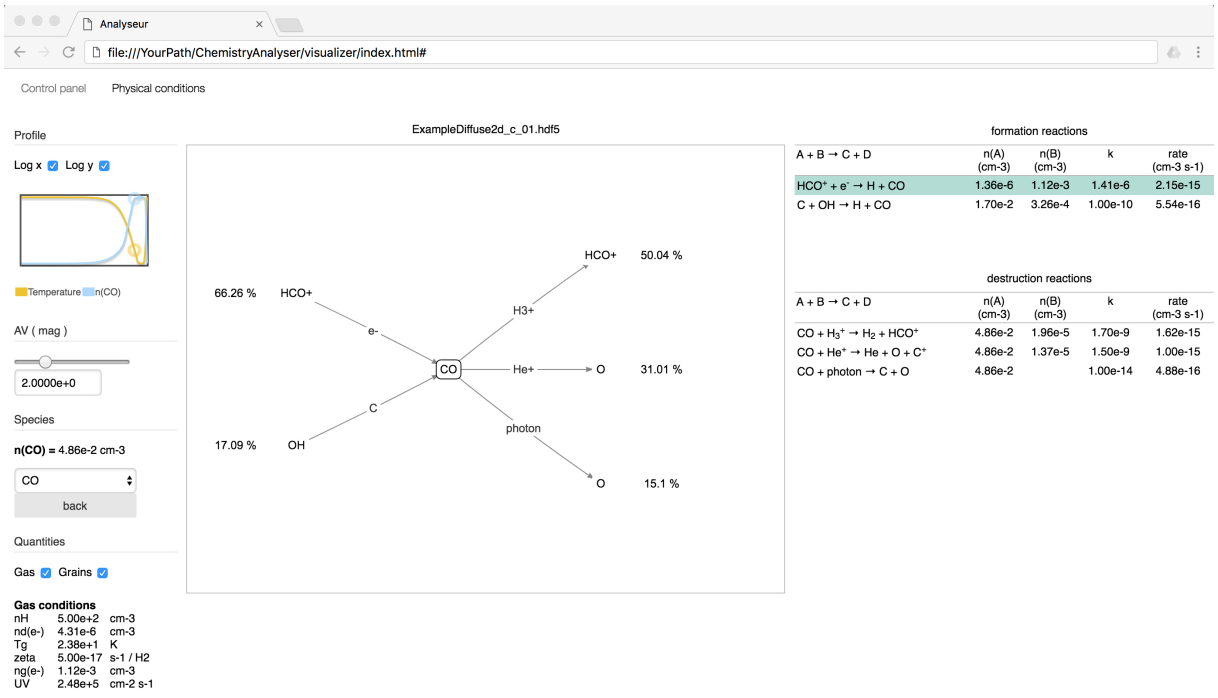

Figure 3.1: Screenshot of the Chemistry analyser tool applied to the output of the PDR model. The graphic shows the main formation and destruction reactions of CO for $A_V = 2$. Useful information concerning gas and dust are accessible on the left with the menu `Physical conditions`. The table below the graph details the values of the reaction rates for all the reactions displayed above.

Physical conditions

4.1 Select a point in the model

By default, the analyser displays the chemical state of the first point of the model. To study a different point, change the value of the main variable with the menu

```
Physical conditions > main variable
```

To facilitate the selection, the profils of the gas temperature and of the density of the selected species are displayed as functions of the model main variable at the top of the `Physical conditions` panel.

4.2 Select another species

Beside clicking on a species in the graph, you can select another atom or molecule `X` with

```
Physical conditions > Species > X
```

or go back to the species you previously studied with the `back` button.

4.3 Getting physical conditions

All information necessary to understand the values / variations of chemical rates are accessible within the software. The gas conditions (e.g. density, intensity of the local radiation field, ...) can be obtained with the option

```
Physical conditions > Gas
```

Dust properties including the densities, charges, and temperatures of grains of different sizes are available with the option

```
Physical conditions > Grains
```