

DOCUMENTATION

Chemistry analyser

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Presentation

The astrochemical models available on the ISM platform 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. 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.

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 / requirements

The Chemistry analyser tool requires python 2.7 and the h5py library. To install these components

- on linux distributions (e.g. ubuntu, debian), we recommend to use the `apt-get` software

```
sudo apt-get install python-h5py
```

- on Mac OS, we recommend `macports` (<https://www.macports.org/install.php>)

```
sudo port selfupdate
sudo port install python27 py27-h5py
```

Beside 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.

2.2 Graphical user interface

The application works with a dedicated internal server. To start this server from a terminal window, go in the `server` directory of the Chemistry analyser tool and type

```
python2.7 server.py
```

Once the server is active, open the `index.html` file located in the `visualizer` directory with any available web browser.

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 occasional 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.

3.4 Extraction of data

The control panel finally allows the user to export data : the reaction scheme, the reaction rate table, 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.

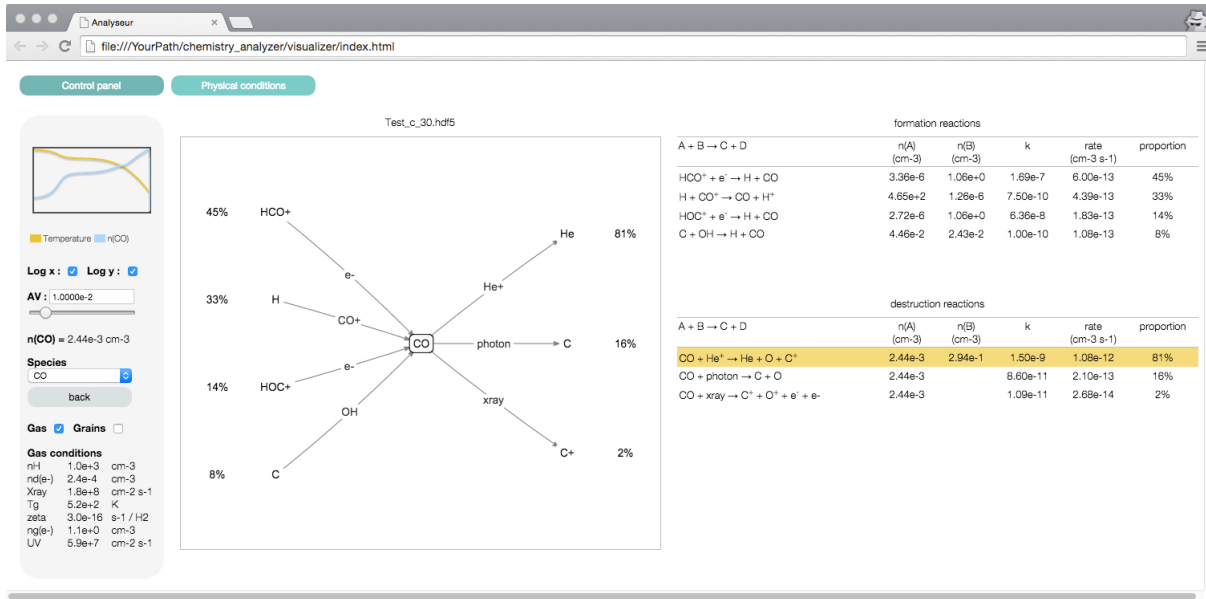


Figure 3.1: Screenshot of the Chemistry analyser tool applied to the output of the PDR model. The graphic shows the main formation and destruction reactions of C^+ for $A_V \sim 0.3$. Useful information concerning gas and dust are accessible on the left with the menu `Physical conditions`. The table 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 profiles 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
```