

MC-ChemDBUI User's Manual

v0.3

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Chapter 1

Introduction

The `mc-chemdbui` graphical interface enables to edit the **MC-ChemDB** database and to generate random samples in **ChemDBPublic** for use in `reactor` (see Fig 1.1).

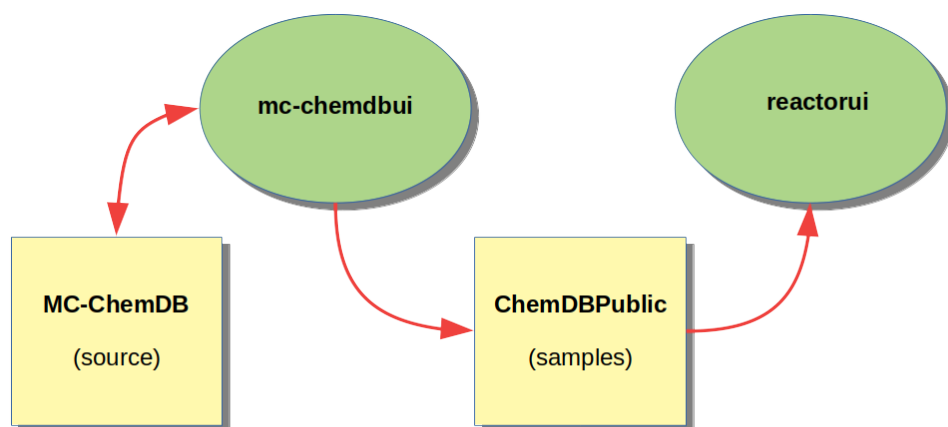


Figure 1.1: Principle scheme of MC-ChemDB.

A good introduction to the data and methods used for uncertainty propagation in the simulation of chemical plasmas can be found in the article

- Z. Peng, N. Carrasco and P. Pernot (2014) “Modeling of synchrotron-based laboratory simulations of Titan’s ionospheric photochemistry”, *GeoResJ* **1-2**:33–53. <http://dx.doi.org/10.1016/j.grj.2014.03.002>

1.1 Installation

1. Load the latest release of **MC-ChemDB** from the GitHub repository <https://github.com/ppernot/MC-ChemDB> and unpack it

2. If it does not exist, create a **ChemDBPublic** directory

3. Download the latest docker container for **mc-chemdbui** from DockerHub

```
docker pull ppernot1/mc-chemdbui
```

4. Run the docker container with source links for **MC-ChemDB** and **ChemDBPublic** pointing to *your* directories

```
docker run -d -p 3820:3820\  
  --mount type=bind,source=path_to_my_ChemDBPublic,target=/ChemDBPublic\  
  --mount type=bind,source=path_to_my_MC-ChemDB,target=/MC-ChemDB\  
  --name mc-chemdbui ppernot1/mc-chemdbui
```

5. Access <http://localhost:3820> in a browser

1.2 Usage

The interface is organized in three modules related to the main **MC-ChemDB** databases:

- **Neutrals module**: manage reactions between neutral species
- **Ions module**: manage reactions involving ions
- Photoprocesses: TBD

Their functionalities are uniformly accessed through a menu with the 'Files', 'Edit', 'Sample', and 'Report' items.

1.3 Curation of MC-ChemDB

If you make changes to the source databases, they will affect your *local* copy only. When these changes are of interest to the community, you have to save them also on GitHub, for instance by creating a fork of the main branch of **MC-ChemDB** (see <https://github.com/ppernot/MC-ChemDB>).

Chapter 2

Neutrals module

2.1 Files tab

2.1.1 Left Panel

This is where one chooses the *version* of the database to load on the **Source DB version** selector. The most recent one is selected by default.

If you want to save changes, you need to type a version tag in the **Target DB version** textbox. The tag might be the same as the source tag, in which case it will be overwritten. Then, press **Save**.

To erase all changes, press on **Restore**.

2.1.2 Right Panel

This panel contains two text editors:

Database It contains the text file (.csv format) in which the database is stored, augmented by an ID column. You can edit the database directly here, but it is not recommended, as the time-stamps will not be managed properly.

Note: If you have important changes to do to the database (such as adding many reactions), it might be simpler to make them directly in the .csv file, before loading it in **mc-chemdbui**.

Release Notes contains the history of the database. You should mention your modifications here. The format is free.

2.2 Edit tab

This panel enables to select individual reactions and display/edit their parameters and rate laws.

2.2.1 Left Panel

The **Edit** tab contains two panels: **Select** and **Plot**.

Select Here, you can filter the reactions by species (as reactant and/or product). The **Reactions** list of filtered or unfiltered reactions can be accessed by a drop-down selector, or navigated using the up and down arrows. If you make changes to the values in the **Right** panel, you

can apply them to the database with the **Apply changes** button. The **Comment reaction** checkbox enables to change the line corresponding to the reaction to a comments line, so it is preserved in the database but not parsed or used to generate samples.

Plot The sliders enable to control the temperature and density ranges for the plots of the reaction rates.

2.2.2 Right Panel

This panel contains the information for the reaction selected in the left panel.

Rate Params All parameters describing the rate law are displayed. You can change them and see the effect on the temperature- and density-dependent plots on the right. Changing the **Reactants** or **Products** fields will create a new reaction. *Warning:* there is no check for double reactions with different parameters. To preserve a change, click on **Apply changes**.

Biblio Presents the list of references mentioned in the reaction's **References** field. The bibtex key links to a notice in the **refDR.bib** file.

Help A short help to the main controls in the page.

2.3 Sample tab

This is where samples of the uncertain reaction rates are generated to be stored in **ChemDBPublic**.

Generate Select the number of samples to generate (typically 500 for production) and **Go!**. This may take some time...

Plot *Mostly used for development control.* Plots of the temperature- and density-dependent reaction rates are generated from the **ChemDBPublic** samples. If everything is OK, they should be similar to the plots in the **Edit** panel.

2.4 Report tab

TBD

Chapter 3

Ions module

3.1 Files tab

3.1.1 Left Panel

This is where one chooses the version of the database to load on the **Source DB version** selector. The most recent one is selected by default.

If you want to save changes, you need to type a version tag in the **Target DB version** textbox. The tag might be the same as the source tag. Then, press **Save**.

To erase all changes, press on **Restore**.

3.1.2 Right Panel

This panel contains two text editors:

1. **Database**. It contains the text file (.csv format) in which the database is stored, augmented by an ID column. You can edit the database directly here, but it is not recommended, as the time-stamps will not be managed properly.
If you have important changes to do to the database, it might be better to make them directly in the .csv file before loading it in **mc-chemdbui**.
2. **Release Notes** contains the history of the database. You should mention your modifications here. The format is free.

3.2 Edit

This panel enables to select and display the parameters and rate laws of individual reactions.

3.2.1 Left Panel

The Edit panel contains two subpanels **Select** and **Plot**.

Select Here, you can filter the reactions by species (as reactant and/or product).

The **Reactions** list of filtered or unfiltered reactions can be accessed by a drop-down selector, or navigated using the up and down arrows.

If you make changes to the values in the Right panel, you can apply them to the database with the **Apply changes** button.

The **Comment reaction** checkbox enables to change the line corresponding to the reaction to a comment line, so it is preserved in the database but not parsed or used to generate samples.

Plot The sliders enable to control the temperature range for the plots of the reaction rate.

3.2.2 Right Panel

This panel contains the information for the reaction selected in the left panel.

Rate All parameters describing the rate law are displayed. You can change them and see the effect on the temperature- and density-dependent plots on the right. Changing the **Reactants** fields will create a new reaction. *Warning:* there is no check for double reactions with different parameters. To preserve a change, click on **Apply changes**.

BRs The branching ratios for multi-channel reactions are displayed here, either as a string (**StringBR**) or as plots. The number of channels in **Nb Channels** has to be consistent with **StringBR**.

Biblio Presents the list of references mentioned **Refs_XXX** fields. The bibtex keys link to a notice in the **refDR.bib** file.

Help A short help to the main controls in the page.

3.3 Sample tab

This is where samples of the uncertain reaction rates are generated to be stored in **ChemDBPublic**. Select **# MC samples**, the number of samples to generate (typically 500 for production) and click on **Sample!**. Options:

Update If this is checked, only those reactions that are newer or have been modified since the last production of samples will be treated. This enables to gain a huge amount of time when slightly modifying an existing version.

Check only No sample is generated. The database is processed and checked for problems in mass balance or species names...

3.4 Report tab

TBD