MC-ChemDBUI User's Manual
v0.4

P. Pernot
pascal.pernot@cnrs.fr

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Chapter 1

Introduction

Simulation of chemical plasmas has to face the important uncertainty of many chemistry parameters, notably on the reaction rates at non-standard temperatures and pressures.[1] Uncertainty quantification (UQ) for the predictions of chemical plasmas models is typically done by Monte Carlo uncertainty propagation (MCUP) where the simulator is run repeatedly for randomly perturbated values of the chemical parameters.

Monte Carlo Uncertainty Propagation is an optimally parallel problem, where an *uncertainty unaware* code of a chemistry model is run repeatedly for different realizations of its uncertain input data. To benefit from this feature and from increasingly available cloud-like computing infrastructures, it is best to keep the uncertainty management separate from the physical model. In the following, one assumes that the uncertain chemistry inputs/databases are provided by a server. This separation has additional advantages for the final user:

- no change to the chemistry code, or minor ones, depending on the uncertainty representation used on the server side;
- no change to the standard format of chemistry files;
- the complex aspects of uncertainty models (*e.g.* for branching ratios) are implemented on the server side.

1.1 The MC-ChemDB system

In this server-client framework, the chemistry server database (`mc-chemdbui`) generates and stores a large number (say 1000) Monte Carlo samples of chemistry files into a public repository (`ChemDBPublic`). Users download a number of these samples according to their needs. The user has then only to run her code on each of the sample to get a sample of model predictions, to be used for uncertainty estimation and sensitivity analysis.

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

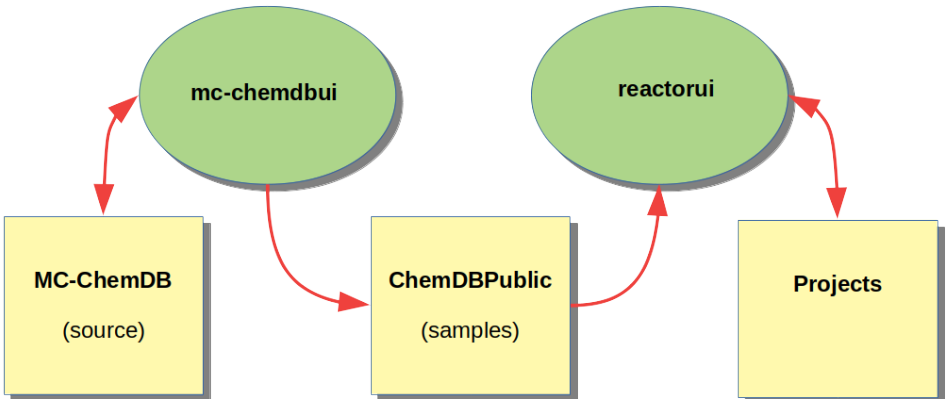

Figure 1.1: Principle scheme of MC-ChemDB ant its articulation with Reactor.

`ChemDBPublic` contains all the chemical reactions encoded in the `MC-ChemDB`. The chemical system under study is specified in `reactorui` which assembles a consistent subset of reactions and extract the relevant data from `ChemDBPublic`.

1.2 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

1.3 Usage

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

- Photo processes: manage photo-processes (photodissociation, photoionization...)

- Neutrals module: manage reactions between neutral species
- Ions module: manage reactions involving ions (ion-neutral collisions, dissociative recombination...)

Their functionalities are uniformly accessed through a menu with the 'Files', 'Edit', and 'Sample' tabs. Each tab contains a `Help` panel describing the main controls.

1.4 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

Photo processes

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 cancel 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 cross-section (XS) and branching ratios (BRs).

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` Various options enable to customize the plots of the cross-sections and branching ratios.

2.2.2 Right Panel

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

`Cross-section` All parameters describing the XS are displayed. You can change the `Data source, Refs and Comments.` To preserve modifications, click on `Apply changes`.

BRs Displays the channels and source of the data. The source cannot be changed, as it is intimately linked to the set of channels described in the database. Such changes are best handled directly in the '.csv' file. The products of each channel can be edited.

`Biblio` Presents the list of references mentioned in the `Refs` 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 XSs and BRs are generated to be stored in `ChemDBPublic`.

Generate Select the number of samples to generate (typically 500 for production), the wavelength resolution(s) and `Go!`. This may take some time... It is possible to perform a blank run by checking `Check only`. The `Sort samples` checkbox affects the generation of BRs. If inactivated, BRs uncertainties are purely random, i.e. there is no wavelength-wise correlations. To introduce some systematic effects (albeit in unknown proportion) one can order the samples for each wavelength and associate them.

Plot Plots of the `ChemDBPublic` samples for XSs and BRs. If everything is OK, they should be similar to the plots in the `Edit` panel.

Chapter 3

Neutrals 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, in which case it will be overwritten. Then, press Save.

To erase all changes, press on `Restore`.

3.1.2 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.

3.2 `Edit` tab

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

3.2.1 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.

3.2.2 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.

3.3 `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.

Chapter 4

Ions module

4.1 `Files` tab

4.1.1 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`.

4.1.2 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.

4.2 Edit

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

4.2.1 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.

4.2.2 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.

4.3 `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...

Bibliography

[1] Z. Peng, N. Carrasco, and P. Pernot. Modeling of synchrotron-based laboratory simulations of Titan's ionospheric photochemistry. *GeoResJ*, 1-2:33–53, 2014. 1