AtChem, an open source box-model for the Master Chemical Mechanism

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Objectives

Box-models are important tools for atmospheric chemistry, used to design, simulate and interpret laboratory experiments and ambient measurements.

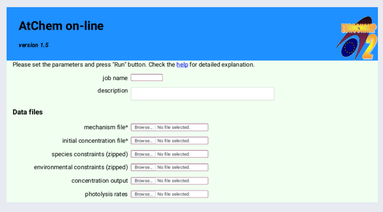
Aim of this work is to develop a box-model for community use with the following requirements:

- Easy to set up and use for novice users.
- Flexible, to adapt to the advanced needs of experienced modellers.
- Suitable for modelling both simple gas kinetics experiments and complex field campaigns.
- Open source: traceability and reproducibility of model results are increasing concerns in the scientific community (e.g., Ince et al. [2012]).

Master Chemical Mechanism (MCM)

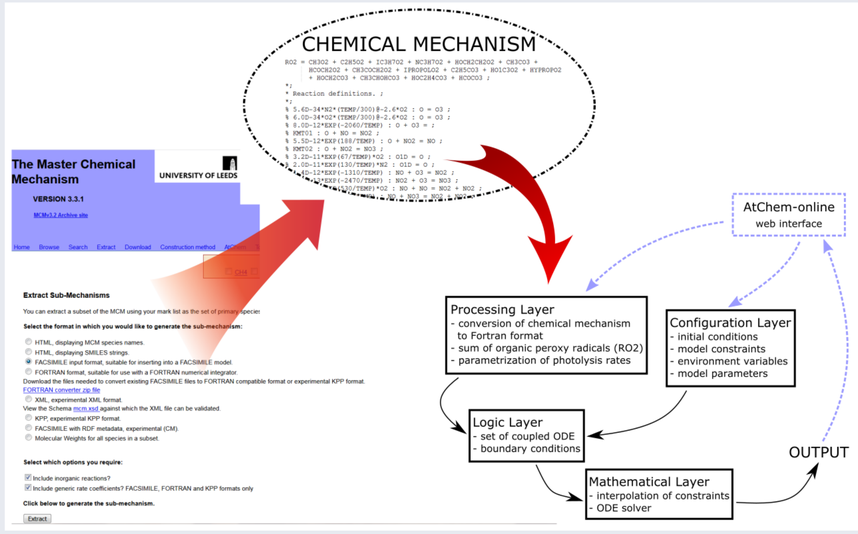
- The MCM is a quasi-explicit chemical mechanism which describes the atmospheric oxidation of methane and 142 non-methane hydrocarbons.
- Available at: `http://mcm.leeds.ac.uk/`.
- Protocol described in Jenkin et al. [1997], updated in Saunders et al. [2003], Jenkin et al. [2015].

AtChem-online



- Developed within the EUROCHAMP2 project.
- Aim: facilitate the use of the MCM to analyze environmental chambers experiments.
- Runs as an online service at: `https://atchem.leeds.ac.uk/`.
- Web interface to aid configuration and running of the model.

AtChem Components



AtChem2

AtChem-online and AtChem2 share the same codebase (rev. 146):

- A modular structure: configuration, processing, logic and mathematical layers. The web interface was removed from AtChem2.
- Integration of the system of differential equations with the CVODE library (part of the SUNDIALS suite, `https://computation.llnl.gov/projects/sundials/`).
- Configuration via simple text files.

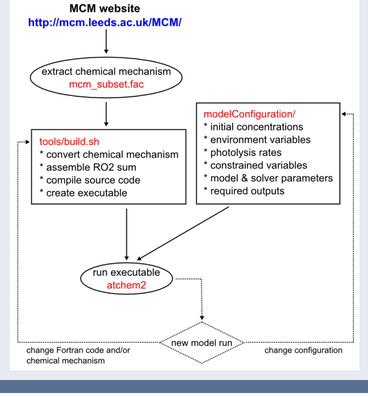
AtChem2 is a major upgrade of Atchem with several improvements:

- Redesigned to be more flexible and sustainable.
- Runs offline ⇒ can be used for more complex models and longer simulations (e.g., field campaigns.) and make use of high performance computing facilities (HPC).
- Modern programming best practices: strict adherence to language standards, version control, continuous integration and extensive testing.
- Easier installation via automated scripts.
- More detailed documentation: `https://github.com/AtChem/AtChem2/wiki`.

AtChem Model Workflow

The design of AtChem makes it easy to set up a box-model, allowing the user to focus on the science questions:

- The chemical mechanism can be downloaded from the MCM website (in FACSIMILE format) and used without modifications.
- The model interpolates the constraints, which can be used directly with their original sampling frequency.
- Changes in the configuration and initial conditions do not require recompilation.



Future Work

- Implement a function parser to facilitate use of the model for sensitivity studies.
- Identify execution bottlenecks and improve integration speed.
- Accept chemical mechanisms in other formats besides FACSIMILE (e.g., KPP).
- Ensure compatibility with MCM/GECKO-A and include TUV calculated photolysis rates.
- Upgrade AtChem-online to the AtChem2 codebase. Develop a new web interface, specifically designed for education and outreach.

Information

AtChem2 is open source, under **MIT licence**.

The current version is v1.1. The code is available on the github repository:
`https://github.com/AtChem/AtChem2`

Installation instructions and documentation can be found on the associated wiki. Contributions, suggestions and feedback are welcome.

Scan me

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