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# AtChem Online Tutorial for EUROCHAMP-2

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- **Run as a free web service using open source software**
- **Core code in Fortran 90**
- **Based on an open-source library CVODE**
- **Uses the same solver as Facsimile**
- **Provides rapid solution of ODE system**
- **Works for any set of differential equations in the correct format**
- **Can use mechanism files downloaded directly from MCM without alteration**



- **Python wrapper:**
  - **uncompresses and prepares the input files,**
  - **runs the simulation on the server ,**
  - **displays the program output and return code,**
  - **provides links to zipped output files.**

# Simple to use



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- **User uploads:**
  - **mechanism file (Facsimile format),**
  - **initial concentrations file,**
  - **some configuration files (*optional*).**
- **User sets environmental variables and model parameters (*opt.*)**
- **User presses “Run”**
  - **simulation runs on the server**
  - **links to input and output files are displayed**



- For this workshop there is an online tutorial with a series of exercises to work through (at your own pace)
- You will need:
  - web browser
  - text editor (e.g. notepad)
  - spreadsheet package such as MS Excel

## Websites

### **Tutorial:**

[http://mcm.leeds.ac.uk/MCM-devel/atchem\\_tut/tutorial\\_intro.htm](http://mcm.leeds.ac.uk/MCM-devel/atchem_tut/tutorial_intro.htm)

**MCM Development site:** <http://mcm.leeds.ac.uk/MCM-devel/home.htm>

**AtChem Online homepage:** <https://atchem.leeds.ac.uk/>



## We need your feedback.

- Difficulty of use: how user friendly is the service?
- Features you would like us to add?
- Tutorial and help page: Are these helpful? Can be improved?
- Will you use AtChem Online in the future?
- Features did you find useful or easy to use?
- How it compares to Facsimile?

**This is *YOUR* community modelling tool, Let us know what *YOU* want!**

*Please fill in feedback form as you work through the tutorial.*