



MEXPLORER-0.0.1

User Manual

The Mechanism Explorer

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Contents

1	Installation	2
2	Input files	2
3	Example usage	2
4	Step 1: Defining the graph	2
5	Step 2: Analysing the reaction mechanism	2
6	Step 3: Graph information and visualization	2

1 Installation

Before installing MEXPLORER, ensure that these pre-requisites are fulfilled:

- necessary: python-3.6
- necessary: graph-tool¹
- optional: CAABA/MECCA²
- optional: skeleton (OIC.dat)

As an alternative to the standalone version of MEXPLORER, it is also available integrated in the CAABA/MECCA atmospheric chemistry boxmodel (since version 4.6.0) in the `caaba/mecca/mexplorer` directory.

2 Input files

information about the chemical mechanism is available in KPP format, as described below.

`mecca.spc`, `mecca.eqn`, `caaba_mecca_rr.nc` (optional), `OIC.dat` (optional)

mechanism in kpp format

Usage via config file `*.ini`

3 Example usage

- List and visualize the species and reactions of the Chapman mechanism:
`mexplorer.py -i chapman.ini`
- Create a file with the methane chemistry in graph-tool xml format:
`mexplorer.py -i CH4_def.ini`
- Plot the most important reactions in the degradation from dimethyl sulfide to SO₂:
`mexplorer.py -i S_DMS_to_SO2_maxflow.ini`
- Plot all reactions in the degradation from dimethyl sulfoxide to SO₂ in the MCM:
`mexplorer.py -i mcm_DMSO_to_SO2.ini`

- Show all species that can produce HCHO within 2 steps:
`info_graph.py -so HCHO,2 simple.xml.gz`
- Show all “primary” species (those that have no precursors) and all “final” species (those that have no sinks) in the MCM:
`info_graph.py mcm.xml.gz -p -f`
- Show all species and reactions in the methane chemistry mechanism:
`info_graph.py -s -r chapman.xml.gz`
- Show all species that are directly produced from isoprene in the MCM, and list the corresponding reactions:
`info_graph.py -si C5H8 mcm.xml.gz`

4 Step 1: Defining the graph

save as a graph-tool compatible xml file

The resulting graph is directly transferred to step 2, and it can also be saved to a `*.xml` file.

5 Step 2: Analysing the reaction mechanism

The resulting graph is directly transferred to step 3, and it can also be saved to a `*.xml` file.

6 Step 3: Graph information and visualization

¹<https://graph-tool.skewed.de>

²<http://www.rolf-sander.net/messy/mecca>