

Hands On Exercises for the Tutorial

(black text: directions; orange text: commands to type or actions to take)

1. Start MusicBox

- a. Open a terminal window and run the following command:
`docker run -p 8000:8000 -it --rm ncar/music-box`
- b. Leaving the terminal window open, open a web browser and navigate to the following address: `localhost:8000`.

2. Start with an Example Chemical Mechanism: Click the “Get started” button

a. Select Chapman Chemistry Example:

Click “Select example” and then select “Chapman Cycle”

b. Review chemical species and reactions:

The page shows the chemical species included that make up the composition of the atmosphere. “M” is simply the sum of all the trace gases.

Click the “Reactions” button to see the Chapman reactions.

Click each reaction to see details about the reaction including the rate constant for Arrhenius and Troe reactions. Photolysis reactions have a “MUSICA name” associated with them so that their values can be prescribed in an evolving conditions file. You can edit the rate reactants, products, yield, and rate constant in the gray box on the right, but don’t do that yet.

Click the drop-down menu at the top of the gray box on right to see the different types of reactions included in MusicBox.

Click “Cancel” button at the bottom of the gray box on right to return to the list of reactions.

Click “Chemical Species” button at top to return to list of trace gases.

c. Review Conditions for running Chapman Chemistry: Click “Conditions” on the left side bar or “model conditions” in the top paragraph.

i. General:

Model options allow you to choose a time step for model integration, a time step for the frequency of printing output, and a length of the simulation. Click on the units of each to see how to change the units.

ii. Initial conditions: Click on “Initial” at the top of the page.

It is possible to upload a file of initial conditions. Let’s do that later. Scroll down to see the initial conditions for the Chapman chemistry example. Note that initial concentrations are in SI units. A unit conversion calculator is available to help with conversion from traditional units or to display values in more traditional units.

Temperature, pressure, and prescribed reaction rate constants can also be assigned here.

iii. Evolving conditions: Click on “Evolving” at the top of the page.

It is possible to upload a file of evolving conditions. This is probably the best way to provide evolving conditions, but let’s do that later.

- d. **Run Model:** Click the “Run Model” button on the left side bar. Three white dots appear while performing the model run. Then an Analysis section is created in the left side bar.
 - e. **Plot Results:** Click the “Plot Results” link Click any trace gas to see its evolution during the model run. Results for O1D, O3, and O2 are shown on the last page. Be sure to display plots with different units: Click units to see drop-down menu.
 - i. *Chemical Species*
Click any trace gas to see its evolution during the model run. Results for O1D, O3, and O2 are shown on the next page.
Click units to see drop-down menu. When you choose another set of units all displayed plots will be converted to the new units.
 - ii. *Reaction Rates*
Click the “Reaction Rates” button at the top of the page and then click any reaction to see its evolution during the model run. Results for O3 photolysis to form O1D and O2 and for the Arrhenius reaction: $O + O_3 \rightarrow O_2$. are shown on the next page.
 - iii. *Environmental conditions*
Click the “Environmental Conditions” button at the top of the page and then click any parameter (air density, pressure, temperature) to see its evolution during the model run.
 - f. **Download configuration files:** Click the “Download” button on the left side bar and then click “Download Configuration File”. A file called “config.zip” will be placed in your Downloads folder. When unzipping the file, a new directory will be created with files describing the model configuration.
 - g. **Download results:** Click the “Download” button on the left side bar and then click “Download Configuration File”. A csv file titled by today’s date and time in UTC (e.g., 2022-04-01 22_15_44.082784_model_output.csv) will be placed in your Downloads folder. The file contains output of both trace gas concentrations (mol m^{-3}) and reaction rates ($\text{mol m}^{-3} \text{s}^{-1}$).
3. **Change the Example – environmental conditions**
 - a. Change temperature and pressure to other values (e.g., 220 K and 3467 Pa (~23 km altitude))
 - b. Run Model
 - c. Plot Results
 4. **Change the Example – initial concentrations**
 - a. Change initial concentrations to other values (e.g., set H2O to 4.5 ppmv)
 - b. Run Model
 - c. Plot Results
 5. **Change the Example – evolving conditions**
 - a. Edit the MusicBox_1_60hPa.csv file
 - b. Upload the file
 - c. Run Model
 - d. Plot Results

6. Add HOx chemistry to Chapman chemistry

$\text{H}_2\text{O} + \text{O}1\text{D} \rightarrow 2 \text{OH}$	$A = 1.63\text{e-}10$	$E_a = -8.28389\text{e-}22$
$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	$A = 1.7\text{e-}12$	$E_a = 1.29781\text{e-}20$
$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2 \text{O}_2$	$A = 1.0\text{e-}14$	$E_a = 6.76518\text{e-}21$
$\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$	$A = 4.8\text{e-}11$	$E_a = -3.45162\text{e-}21$

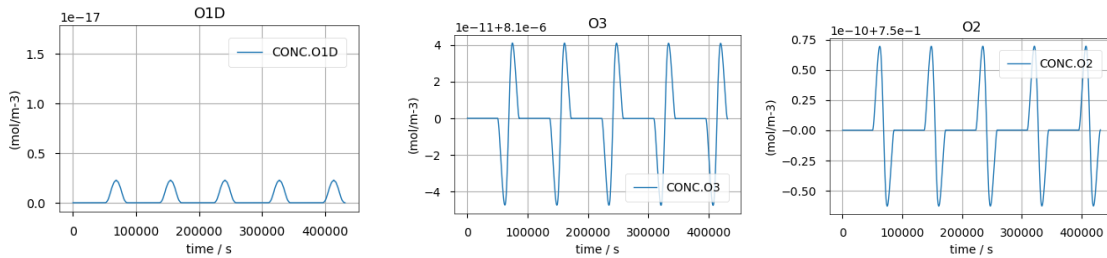
- a. Add OH and HO₂ to the list of chemical species:
 - Click on “Mechanism” in the left sidebar.
 - Click on “Add species” button.
 - Type in species name (e.g., OH)
 - Click on “property value” and provide molecular weight (OH 17 g/mol, HO₂ 33 g/mol – look at units!)
 - Click “Save”
 - Repeat for other species.
- b. Add reactions for OH and HO₂
 - Click on “Reactions” button at top and then click on “Add reaction” button
 - Select type of reaction (e.g., Arrhenius)
 - Add reactants and products (e.g., OH + O₃ → HO₂ + O₂). These are done with drop-down menus.
 - Add reaction rate according to formula provided ($A = 1.7\text{e-}12$, $E_a = 1.29781\text{e-}20$)
 - Click “Save”
 - Repeat for other reactions
- c. Add initial concentrations for OH and HO₂, if desired
 - Click on “Conditions” and then “Add”
 - Select species and provide initial concentration in mol m⁻³
 - Click “Save”
- d. Run model
- e. Plot results
- f. Download the configuration file
 - Your newly created mechanism is now saved to your computer.
- g. You can use it the next time you work with MusicBox by uploading the files.
 - Click on “Start Here” and then “Load configuration file”.
 - Select the zip file that you want to upload and click “Upload”.

A full stratosphere chemistry mechanism is available in the repository.

Click “Start Here” and then visit “this repository” written in the paragraph.
Click the “Stratospheric Mechanisms” folder, then the “Full_Chapman” folder.
Click on one of the folders (e.g. 20km_Strat_Mechanism).
Click on the zip file (e.g., 20km_Strat__Full_Mechanism.zip)
Click on the “Download” button. Unzip the file in your Downloads folder. The zip file can then be uploaded to MusicBox interactive.

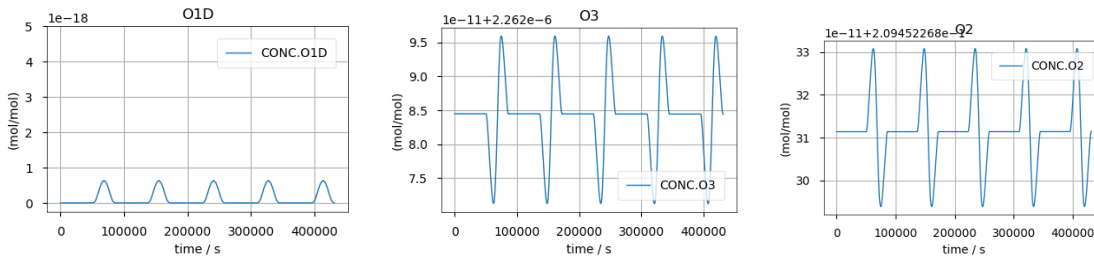
1. Plot Results – Default Chapman Chemistry

a. Chemical Species: Results in the SI units mol/m³:

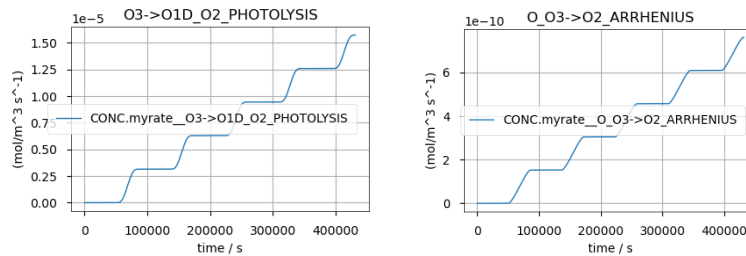


Note that O3 and O2 are displayed as the difference from their initial values. That's why there are negative values.

Results in mol/mol:



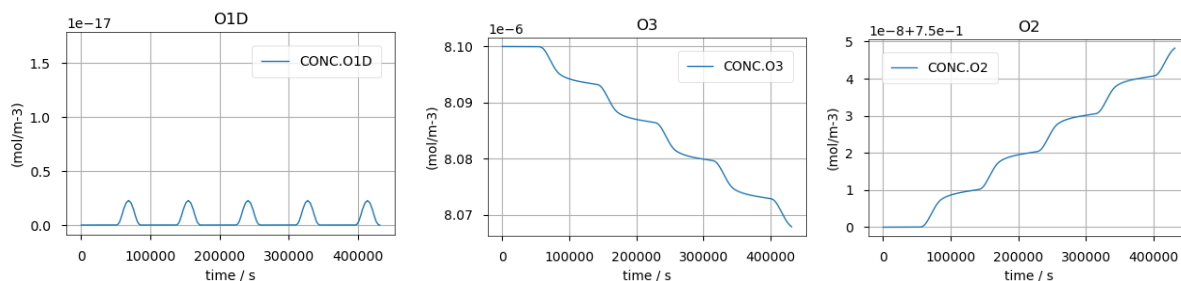
b. Reaction Rates: Results are in SI units (mol m⁻³ s⁻¹)



The title of the plot describes the reaction. For example, the left plot is for O3 photolysis to form O1D and O2. The right plot is for the Arrhenius reaction: $O + O_3 \rightarrow O_2$.

2. Plot Results – Chapman Chemistry with HOx reactions

a. Chemical Species: Results in the SI units mol/m³:



Note the O3 loss and O2 production (O2 is displayed as the difference from its initial values). Here are the results for OH and HO2:

