Running RMG Jobs Exercise

There are many example RMG input files in `RMG-Py/examples/rmg/` (https://github.com/ReactionMechanismGenerator/RMG-Py/tree/main/examples/rmg) folders on RMG-Py GitHub that have different settings and reaction systems. For this exercise, try running 'minimal' example using the 'minimal_input.py' input file located in this folder.

Step 1: Run the input file

1. Open the terminal in the folder that contains the 'minimal_input.py' file.
2. Activate rmg_env by typing the below line on your terminal

   ```
   conda activate rmg_env
   ```

   If it fails, try the below line instead

   ```
   source activate rmg_env
   ```

3. The command you use for running a RMG input file using the RMG binary follows the format:

   ```
   rmg.py path_to_your_input_file/input_file_name.py
   ```

   where `path_to_your_input_file` is a path to the folder that contains your input file and 'input_file_name' is the name of your RMG input file.

   Since you are already in the folder containing the input file, you can simply type the line below to run the RMG input file.

   ```
   rmg.py minimal_input.py
   ```

The minimal example should take only a few minutes to finish. If it ran successfully, you should be able to see the following messages at the end (termination time will be different). Depending on the version of RMG used, the final model core and edge sizes might be different:

```
MODEL GENERATION COMPLETED

The final model core has 26 species and 71 reactions
The final model edge has 175 species and 391 reactions

RMG execution terminated at Mon Aug  8 18:27:42 2022
```

If the RMG simulation is taking too long, you can stop it by pressing ctrl + z.

Step 2: Explore the output files

If your RMG job ran successfully, you will see various output files in your folder. Even if you terminated your job in the middle of simulation, you will still find various intermediate output files in your folder. Let's take a look at the chemkin file result using one of RMG-website tools.

1. Click "Visualize Chemkin File" tool in the RMG Tools page (https://rmg.mit.edu/tools/)
2. Click "Choose File" under "Chemkin File" and select "`chem_annotated.inp`" file that is created under "chemkin" folder.
3. Click "Choose File" under "RMG Dictionary" and select "`species_dictionary.txt`" file that is created under "chemkin" folder.
4. Click "Submit" and wait. If "Click here for your generated output file" line appears, click it to visualize the Chemkin output files.
5. Scroll down to see the results.