Methane Combustion Exercise

We will modify the given "`input.py`" file to simulate a simple methane combustion model. We want to include methane and oxygen as reacting species with 1:2 (methane : oxygen) initial mole fraction ratio and simulate the simpleReactor at 1350 K and 1 bar until we reach 90 % conversion of methane or reach termination time of 1e6 seconds.

Tip: you can use RMG's molecule search tool to look up species SMILES.
https://rmg.mit.edu/molecule_search

Step 1: Modify the RMG input file

1. Open the provided '`input.py`' file with any text editor you prefer (e.g. Notepadd++).
2. Edit 'species' line to change 'ethane' to 'methane'. Make sure you change the SMILES to methane SMILES as well. Add 'oxygen' as a second species. Use RMG's molecule search tool if you want to look up species SMILES. Make sure you are using oxygen SMILES with multiplicity 3.
3. Edit 'simpleReactor' line by setting the mole fractions of 'methane' and 'oxygen' to 0.33 and 0.67, respectively. Set 'terminationCoversion' of 'methane' to 0.9.

Step 2: Run the input file (not until it finishes)

1. Open the terminal in the folder that contains the '`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 below:

   ```
   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 input.py
   ```

4. This RMG job might take too long to run on a local computer (~30 min), so you do not need to run it until it finishes. Terminate the RMG job early by pressing ctrl + z on your terminal if it is taking more than ~5 minutes.

If it ran successfully until the end, 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 58 species and 289 reactions
The final model edge has 1108 species and 2337 reactions

RMG execution terminated at Tue Aug  9 17:04:01 2022
```

Step 3: 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, you will still find various intermediate output files in your folder if the RMG job ran up to certain extent. 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.