RMG Liquid Reactor Exercise

In this exercise, we will modify the example liquid phase reaction that can be found in `RMG-Py/examples/rmg/liquid_phase/` and run it with a different solvent. The original input file simulates the autoxidation of 'octane'. We will change the solvent to 'pentane' instead.

Tip1: You can use RMG's molecule search tool to look up species SMILES.
https://rmg.mit.edu/molecule_search
Tip2: You can use RMG's solvent library tool to look up a list of solvents.
https://rmg.mit.edu/database/solvation/libraries/solvent/
You can also search a solvent using RMG's solvent search tool.
https://rmg.mit.edu/database/solvation/solventSearch/

Note on available solvents in RMG: When you find the solvent of your interest on RMG-website, make sure that all "Abraham parameters", "Mintz parameters", and "Viscosity parameters" are available. If any of them are not available, you cannot use that solvent for RMG liquid phase simulation.

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 'octane' to 'pentane'. Make sure you change the SMILES to pentane SMILES as well. Use RMG's molecule search tool if you want to look up species SMILES.
3. Edit 'liquidReactor' line by changing 'octane' to 'pentane'. You can keep the rest same.
4. Edit 'solvation' line by changing a solvent from 'octane' to 'pentane'.

Step 2: Run the input file

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
```

This RMG job 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 16 species and 33 reactions
The final model edge has 115 species and 479 reactions

RMG execution terminated at Tue Aug  9 00:10:18 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.