Running RMG Job Exercise – Oxidation of exhaust gas emissions

Download the input.py file from GitHub
https://github.com/yunsiechung/RMG_workshop/tree/main/RMG_exercises

Step 1: Open the input file

1. The input species are CO_2, H_2, CH_4, H_2O, CO, N_2, O_2
2. We want to investigate Pt(111) as the active site, which we simply define by the following command:
    a. catalystProperties(metal = 'Pt111')
3. The reaction library 'Surface/CPOX_Pt/Deutschmann2006' is loaded
4. Conditions for the mechanism generation (we use a reactor with a temperature range, using nSims=3)
    a. T=600-973 K, p=1 bar
    b. Initial mole fractions
        i. H_2= 0.167 %
        ii. CO_2=12 %
        iii. H2O=12 %
        iv. CO=0.5%
        v. CH4=0.3%
        vi. O2=0.9335%
        vii. N2=74.0995%
    c. Termination rate ratio: 1e-10

Step 1: Run the input file

5. Open the terminal in the folder that contains the '`input.py`' file.
6. Activate rmg_env by typing the below line on your terminal

```
conda activate rmg_env
```

7. 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
```

The minimal example should take 2 minutes to finish. If it ran successfully, you should be able to see the following messages at the end (termination time will be different):

```
MODEL GENERATION COMPLETED

The final model core has 24 species and 46 reactions
The final model edge has 37 species and 101 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

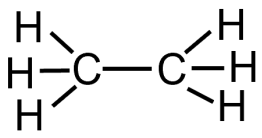
If your RMG job ran successfully, you will see various output files in your folder like this. Let's look at some of the results.

1. Open the folder "Solver" and look at the last produced image. What are the main products?
2. Open the output.html and output_edge.html file. Explore the discovered species and reactions.

Step 3: Modify the input file

Now it's your time to play around with the input file to see how the mechanism and the generation procedure changes.

1. Change the temperature by +100 or -100 K. How does this affect the speed of the generation and the discovered mechanism?
2. Change the metal. You can choose between Co0001, Ag111, Au111, Ru0001, Cu111, Ni111, Pd111. For some of these metals it might take very long. If it takes too long abort the generation by pressing ctrl + z.
3. Add 0.5% of ethane (C2H6) as a reactant. You need to provide the adjacency list for this molecule and add the concentration in the reactor. The Lewis structure is the following:



Use the adjacencyList of O_2 as an example. Remember the following:

a. u is the number of free unpaired electrons for each atom
b. p is the number of free electron pairs
c. c is the charge

Here is a start for the adjacencyList. You need to fill in all the bonds.

```
C2H6
1 C u0 p0 c0 {2,S}
2 C u0 p0 c0
3 H u0 p0 c0
4 H u0 p0 c0
5 H u0 p0 c0
6 H u0 p0 c0
7 H u0 p0 c0
8 H u0 p0 c0
```

If you cannot create the adjacencyList, you can look at the solution folder.