Argon adsorption in carbon nanotube

Project for Nanoengineering classes. Deadline: June 15th, 2020.

Perform Grand Canonical Monte Carlo (GCMC) simulations of adsorption and desorption of argon in single wall carbon nanotubes of different diameters.

Run the simulation of argon adsorption in carbon nanotubes at boiling temperature of argon. Prepare adsorption isotherm for pressures up to $0.2\ p_0$, where p_0 is a saturation pressure for argon in desired temperature (https://bit.ly/2XmpXO6). Use attached structures of carbon nanotubes with diameters between 10 Å and 40 Å.

What types of pore are represented by structures with different diameters?

Please make sure that you have

force_field_mixing_rulex.def,
pseudo_atoms.def,
ar.def,
simulation.input

files in your working directories and that they are properly formatted. There are some XXX parameters which you need to change. That includes:

- simulation.input:
  - Number or initialization and production cycles (try 2000 and 2000, respectively, as the first attempt)
  - Frequency of printing of the system properties (useful for equilibration checks)
  - Framework name (same as .cif file name)
  - Multiplication of the unit cells (remember that that in each direction, the length of the cell should be larger than doubled interactions cutoff)
  - Temperature of simulations (Ar boiling temp.)
  - Pressures of simulations (several points, up to approx. $0.4\ p_0$)
  - Frequency of writing of the movies
  - Probabilities
- force_field_mixing_rulex.def:
  - Number of defined interactions
  - Interactions parameters ε and σ for argon (you can find it in argon.pdf file, in Table 2.) and carbon (you can find it in cnt.pdf file, in Table 2). IMPORTANT parameters must be provided in units of Kelvin and Angstrom, respectively.
- pseudo_atoms.def:
  - mass and charge of atoms

In the simulation.input file you will find additional block that restricts the moves to a cylinder to prevent adsorption of molecules outside of the nanotubes. It includes the definition of direction, center in fractional coordinates, and radius of the cylinder:

```
Cylinder                    0
CylinderDirection           Y
CylinderCenter              0.5 0 0.5
CylinderRadius              X
```

Prepare plot with adsorption and desorption isotherms for different carbon nanotubes (use $cm^3(STP)/g$ units). To simulate desorption isotherm, you need to copy restart file from the highest pressure to a `RestartInitial/System_0/` folder, add `RestartFile yes` keyword in the 5th line of the input file, change (reverse) the range of the pressures and run the simulations again (prior to that either change the name of the adsorption outputs or copy them to different directory, otherwise you may lose the adsorption data because they will be overwritten).

You can use command:

```
mkdir des;cp * des/;cp -r Restart/ des/;mv des/Restart/ des/RestartInitial
```

to create folder for desorption simulation. However, you still need to modify the input file.

Include the error bars. If the error bars are large, **check the fluctuations of the number of molecules and energy and plot it**. **What is the potential source of large errors?**

If your simulations will not be finished by the date of the deadline (some of the high pressures in largest structure runs may be long), instead of extracting the `Average loading absolute [cm^3 (STP)/gr framework]` from the end of the output file, **use averaged amount of adsorbed molecules from the fluctuations and include fluctuations vs. MC cycles plot. Explain this in the final report.**

What types of isotherm and hysteresis did you obtain? **Why isotherms for different diameters are different**. **Interpret parts of isotherms (increases and flattening), and what happens with adsorbed molecules at particular pressures**. Looking at the movies should be helpful. It is also good to plot the isotherm both in linear and log scales.

Submit the results as a report file in PDF format, name it `name_lastname.pdf`.