Starch composite Hydrogels for Waste-Water Treatment

DISA- Design Innovation Summer Award

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Proposed By :

I. Rohan Yuttham (2017ME10605)
II. Arpit Agrawal (2017ME10566)
III. Aman Kumar (2017CH10196)

Under the supervision of:

Dr. Gaurav Goel

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Abstract

The central goal of the project was to study the interaction between Thermo-plastic starch, water, and clay Nano-particles in a simulated environment.

To achieve this goal, we worked with the software namely,

- Gromacs
- Packmol
- Pymol

The duration of the project was 8 weeks during the month of May to July.

Excerpt of the work done in the project

1. Prepared a correct topology file of Thermo-Plastic Starch(TPS) from available coordinate files of
   - Amylose,
   - Amylopectin, and
   - Sorbitol.

   From previous research work done we had the composition of TPS as –

Compounds	#mols
Amylose	90
Amylopectin	42
Sorbitol	4633
Water in Charmm36	256X13 =3240

And we get the weight of TPS=W_i= $1.34X10^{-21}$g

2. To accomplish our task, we required to make a hydrogel system with percentage composition(w/w) as-

a. TPS-10%
b. Water-90%

3. Now we aimed to prepare the final hydrogel in a cubic box of side length $15\ nm$ equivalent to volume of $3375 nm^3$.

We were expecting a density less than $1.1\ g/cm^3$ and greater than $1\ g/cm^3$.

So, we needed to find the **weight of thermos-plastic starch** using the above data.

Calculation:

Assume total weight of system as 'x' gram.

Then, Weight of TPS= 0.1'x' gm

Its density= 1.34 gm/cm^3

Its volume = $(0.1x/1.34)\ cm^3$

Weight of water= .9x gm

Its density= $1 gm/cm^3$

Its volume = $0.9x\ cm^3$

So, total volume = $0.975x\ cm^3$

Equating it to 3375 nm^3 => Weight of TPS (x)=W_n = 0.3462 X 10^{-18}g
Which gives W_n/W_i = 0.08

Maintaining this ratio of weights calculated from above data, the new number of moles will be 0.08 times the previous one-

This gives:

Compounds	#mols
Amylopectin	3
Amylose	7
Sorbitol	371
Water	1X256

Total mass (from gromacs) : 445722.081 amu

4. Now we packed these molecules using the software "Packmol".

The output is a .pdb file.

5. Next ,we prepared a correct topology of TPS.
We used 'pdb2gmx' and edited the topol.top file according to our need.

6. Begin with simulations in Gromacs.

7. First step is solvation of the box.
   i. Command used- gmx solvate.

   Results:

   a. Volume- 3375 nm^3
   b. Density- 1.097 gm/cm^3

8. Secondly, Energy Minimization of the solvated system
   The parameters are given in minim.mdp[1].

9. It was followed by NVT and NPT steps. The parameters are given in nvt.mdp[2] and npt.mdp[3] respectively.

10. After completion of the two equilibration phases, the system was well-equilibrated at the desired temperature and pressure.

11. We are now ready to release the position restraints and run production MD for data collection. The script is given in md.mdp[4].

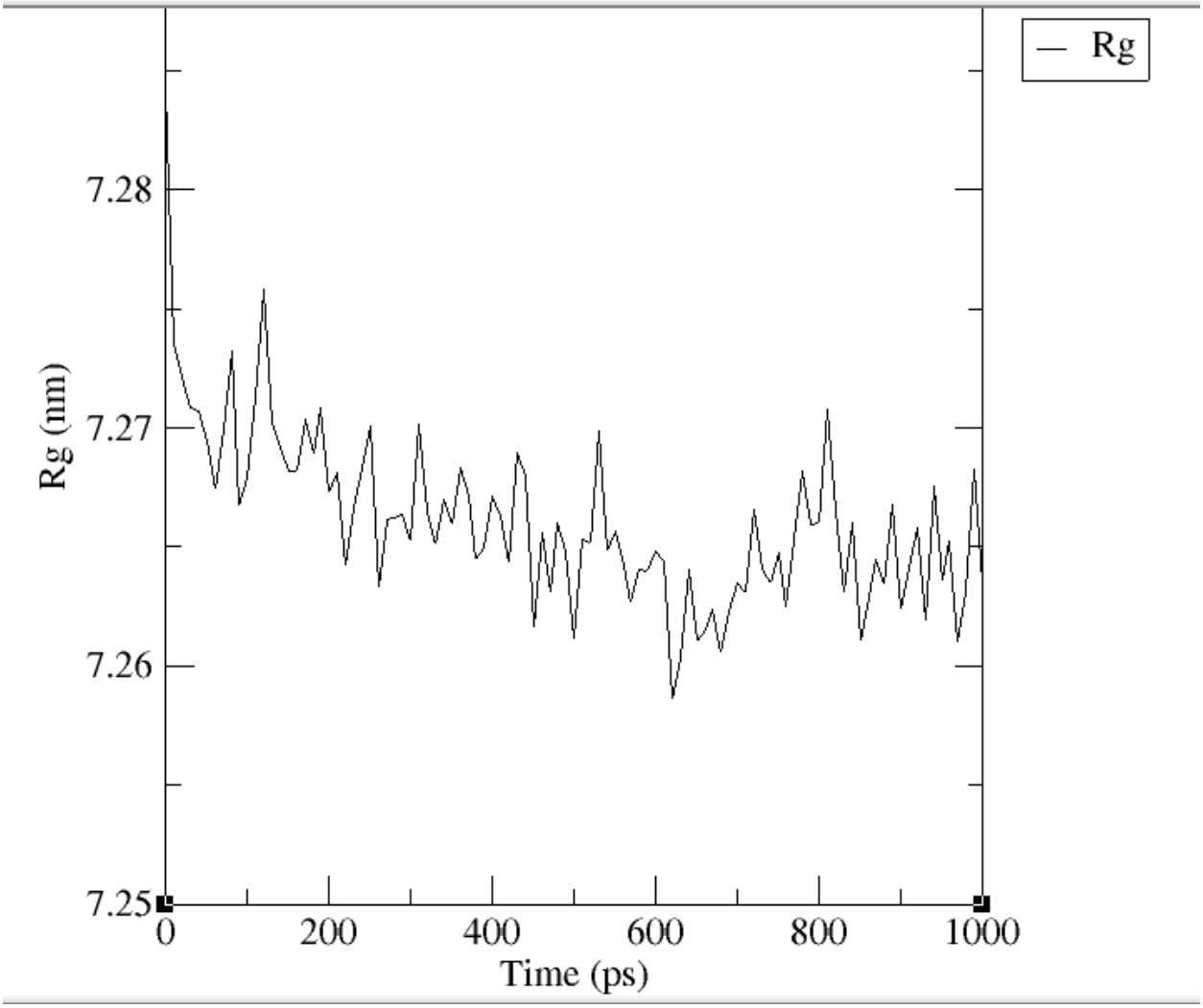
Finally we got a md_0_1.gro file and other associated files with it.

Note: that the temperature, pressure, simulation time and other parameters are stored in the .mdp script. The parameters were decided based on discussions with seniors.

Analysis

- Radius of Gyration

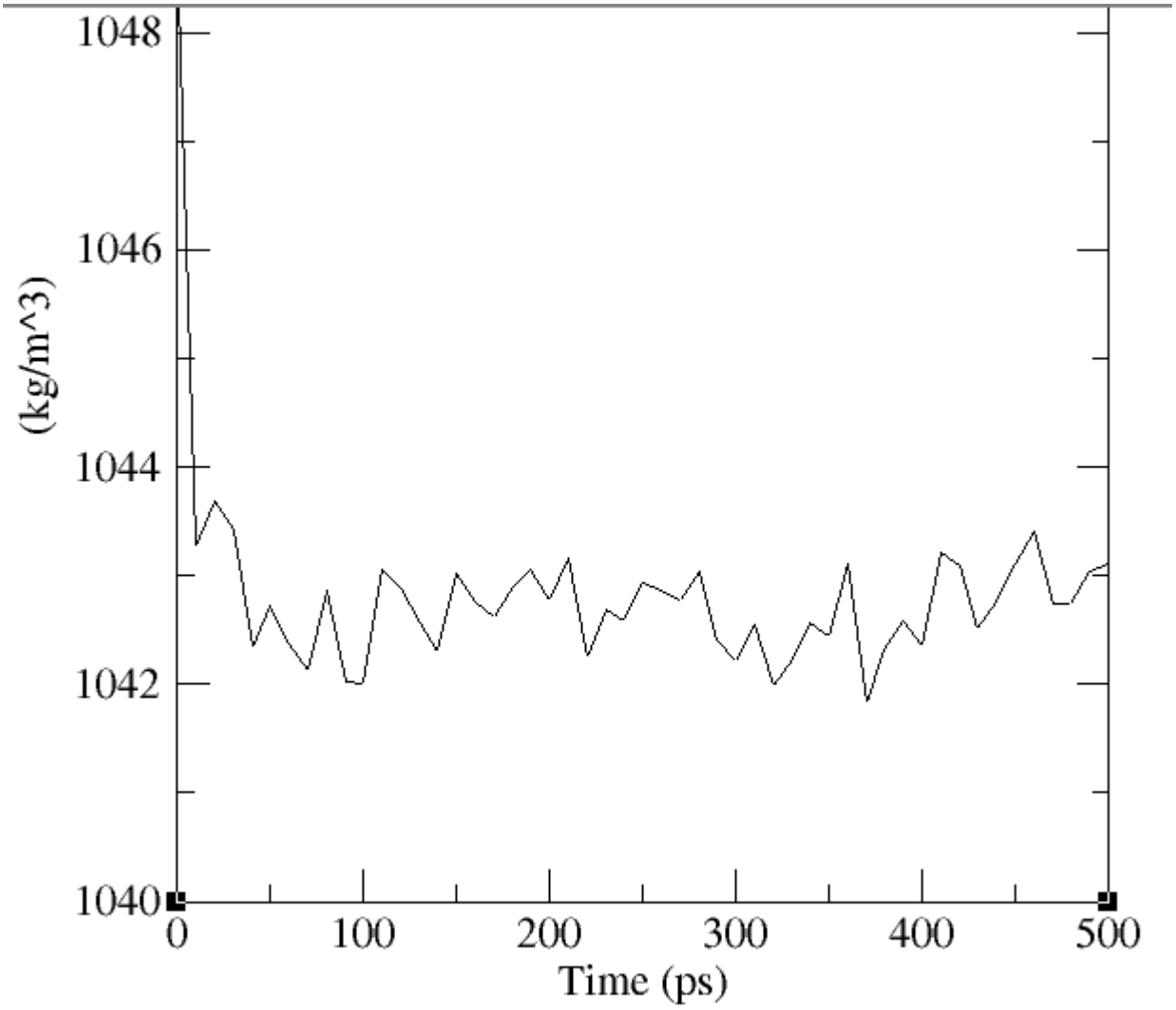
The R_g is plotted against time as



* The radius of gyration of a protein is a measure of its compactness. If a protein is stably folded, it will likely maintain a relatively steady value of Rg. If a protein unfolds, its Rg will change over time.

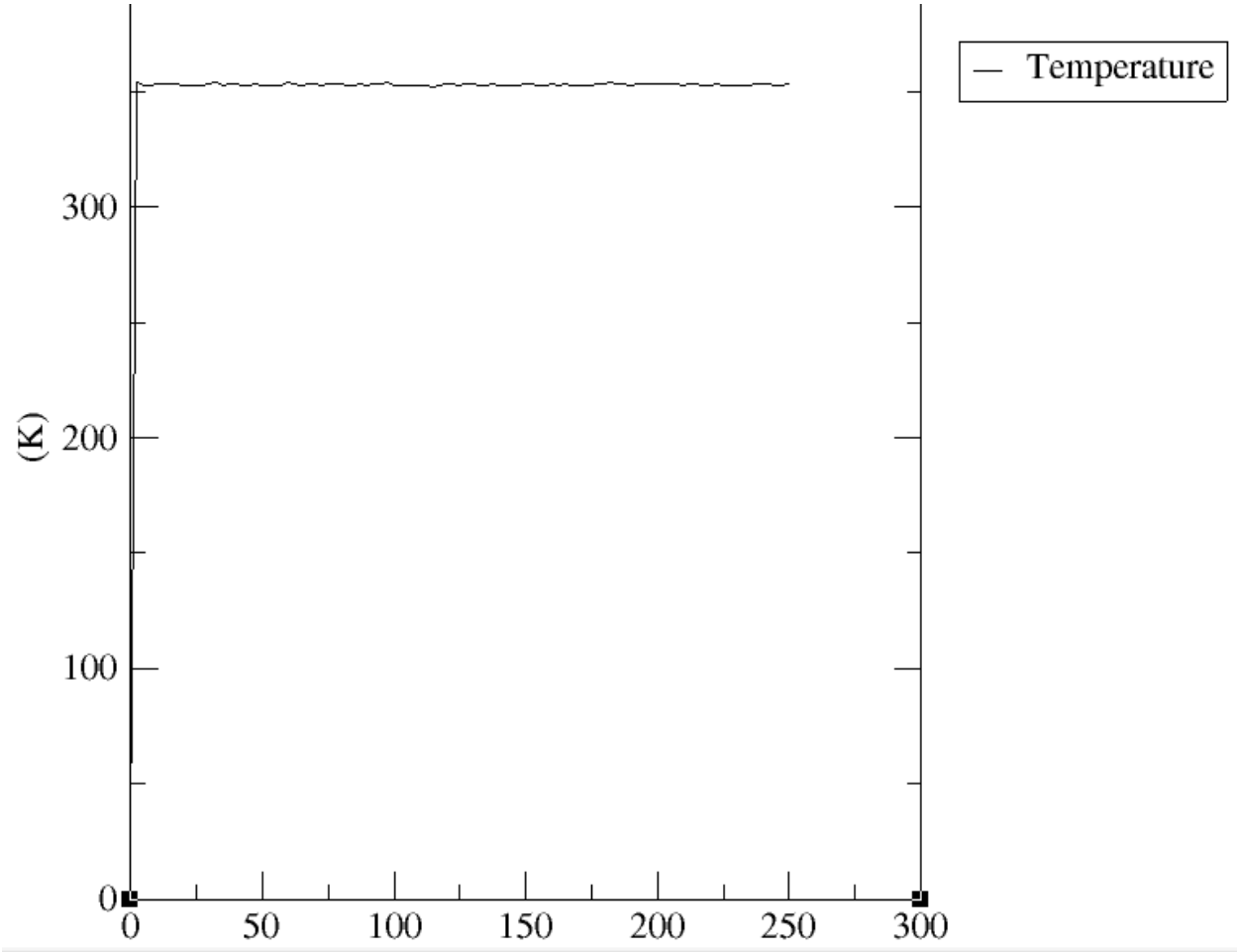
- Density

The density is plotted against time as



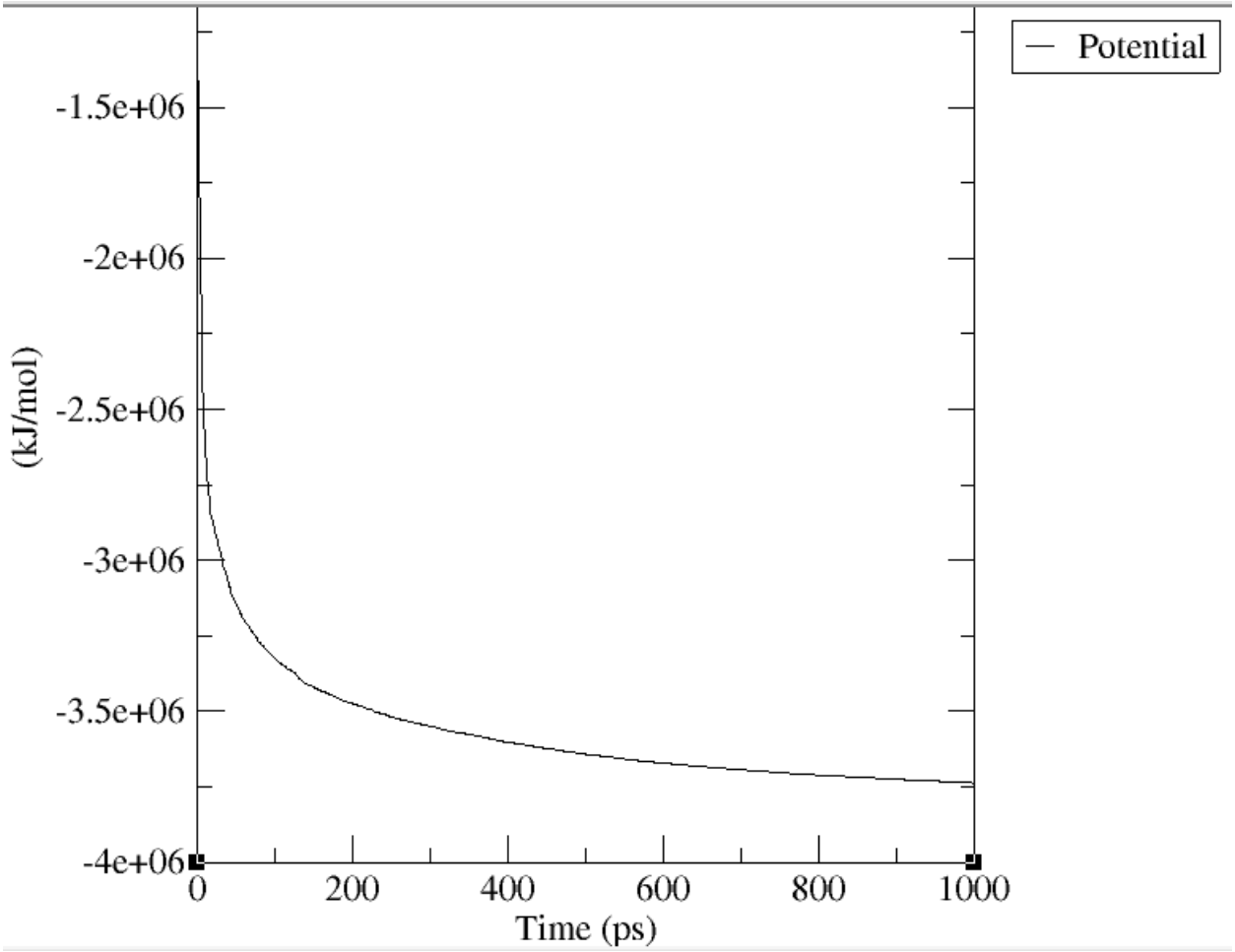
- Temperature

The temperature is plotted against time as



- Potential

The potential is plotted against time as



- The box size being small, some chains might have been incomplete due to finite chain length.
- So, we did new simulation with a cubical box having side length 23nm.

By calculating no of chains from the method mentioned above, required no of chains are:

compounds	**#chains**
amylose	21
amylopectin	10
sorbitol	1066

- After this the box was solvated with water molecule and performed the energy minimization ,nvt, npt simulations in the similar way.
- This system was much more feasible than the 15nm system due to optimized parameters.

*The files of the above system are also attached.

Future aspects and conclusion

- The equilibrated system of the hydrogel prepared can be used as an adsorbent when simulated with clay nanoparticles with the clay nanoparticles and heavy metals behaving as adsorbates.

- The surface of clay MMT can adsorb certain heavy metal particles on its surface.