

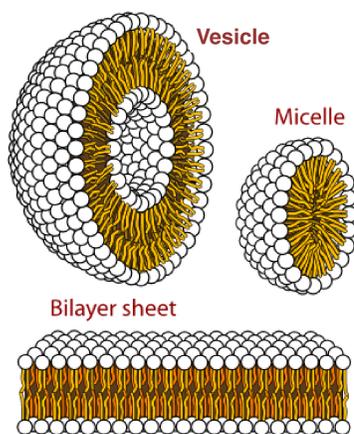
## Abstract

Span 80, also known as sorbitan monooleate, is an inexpensive, biocompatible amphiphile molecule with properties similar to a typical surfactant. It consists of a hydrophilic head made of several hydroxides and a long, hydrophobic tail made up of carbons. When several of these molecules are added to an aqueous solution, there is a tendency for the molecules to begin clustering, forming various structures such as micelles and vesicles, which allows the hydrophobic tails to be surrounded by the hydrophilic heads. With the help of Molecular Dynamics, using programs such as GROMACS<sup>[1]</sup> and VMD<sup>[2]</sup>, we were able to analyze the clustering effect of many molecules of span 80 over a time interval of just under 30 nanoseconds.

After about half of a nanosecond there were just fewer than ten mini-structures or amphiphiles and by 6 nanoseconds they had merged to form one definite structure or micelle. This was fairly early in the simulation so there is a possibility that some vesicles may have formed towards the end. Using VMD, it is possible to zoom into the middle of the final structure and highlight several water molecules within the center of the vesicle.

## Background

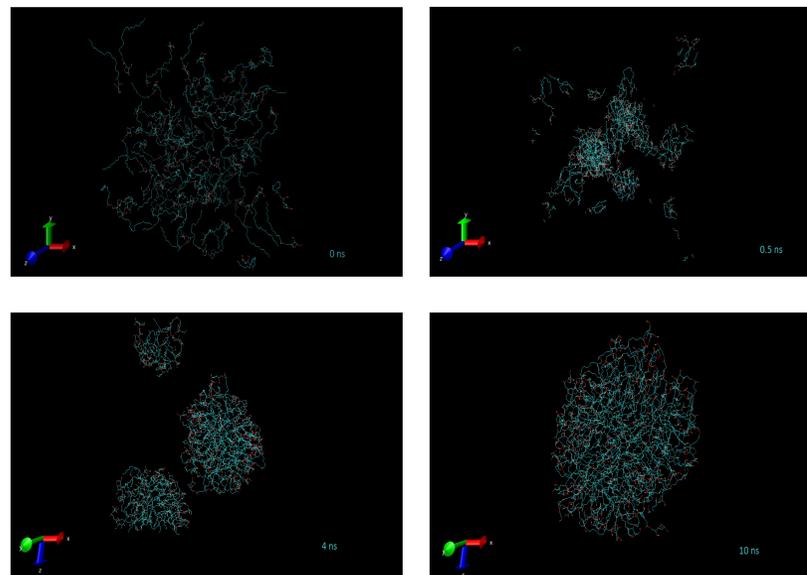
Span 80 is found in various products, and is typically used in cosmetics or in prescription drugs as a drug carrier. When placed into an aqueous solution, ideally it begins to cluster into a micelle, which is basically a sphere where the hydrophilic heads are on the outside and the hydrophobic tails are on the inside. When it sits in this aqueous solution for longer periods of time, we can begin to see the formation of vesicles, which, like a micelle, is a sphere with the heads on the outside and tails on the inside, but on the inside there is another layer of the heads and inside that is more water (refer to figure 1). This structure is useful as a drug carrier because certain drugs, e.g. Vitamin E, can be placed inside, allowing it to travel further into the digestive system before being dissolved into the blood stream.



**Figure 1:** Several basic structures a typical surfactant (such as Span 80) can form.

## Analysis

Figures 2 depict the time evolution of the simulation system. At  $t = 0$  the Span 80 molecules were set up to be spread evenly in the simulation box so that there were no large clusters and only large number of smaller aggregates at the starting time. Quickly, however, this number drops from 70 to below 10 within the first 0.5 nanoseconds. Then it proceeds to gradually decrease towards one larger cluster until about 5 nanoseconds and remains at one until the end of our 28 nanoseconds of simulation. This shows that the rate at which they cluster is much higher at the beginning than it is at the end. So what does it do for the last 20 nanoseconds of the simulation? Visual analysis suggests that the cluster organizes itself as a vesicle (refer to background). Using VMD, we were able to locate a few water molecules within the structure, showing evidence that it is possible that the building of this vesicle may have initialized.



**Figure 2:** Several snapshots of the simulation system.

## Simulation Methodology

- Set up the initial structure, from files with the coordinates of atoms in each type of molecule, using packmol
- Ran energy minimization on the initial structure to get an equilibrium state.
- Set up run script to include: which directory to find specific files, where to put the output files, what program to use (GROMACS in our case)
- Submit job to super computer

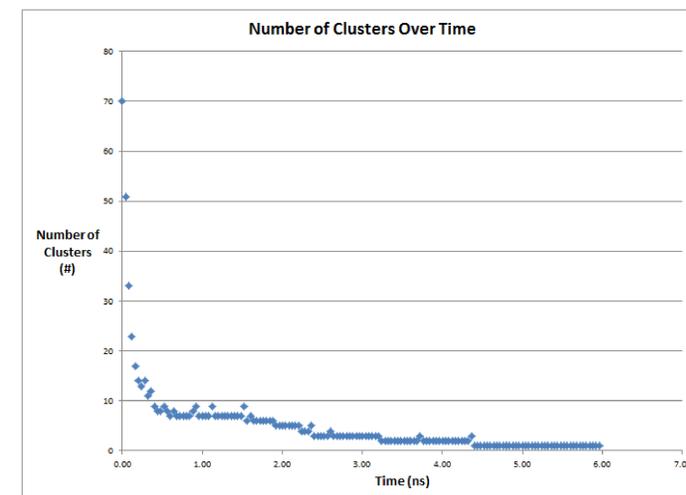
## References

- [1] Groningen Machine for Chemical Simulations (GROMACS) - <http://www.gromacs.org/>  
 [2] Visual Molecular Dynamics (VMD) - <http://www.ks.uiuc.edu/Research/vmd/>

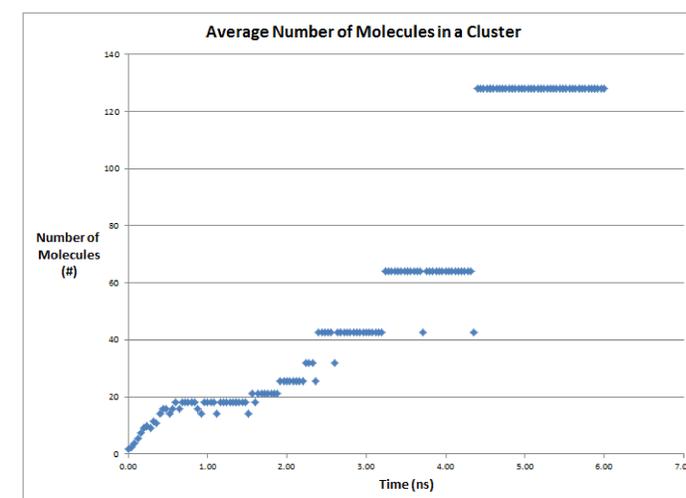
## Conclusion

The goal of this project was to learn about molecular dynamics simulation methodology and to apply this knowledge to study the self-assembly of Span80 molecules in water. After preparing and running the simulation using GROMACS, we visualized the simulation results using VMD package. Using other functions of GROMACS we were able to quantify the clustering in time of the Span 80 molecules. Graph 1 shows the total number of clusters as a function of simulation time. The clustering process is completed in about 6 nanoseconds. Graph 2 shows the average number of molecules that are part of a given cluster. The two graphs are consistent with each other as for example, at times when there is just one cluster in the system the average number of molecules is 128 (which is the total number of molecules). At times when there are two clusters in the system there are, on average, about 64 molecules per cluster, and the process goes on.

**Graph 1**



**Graph 2**



## Acknowledgements

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