Generating Phase Diagrams via HLD-NAC

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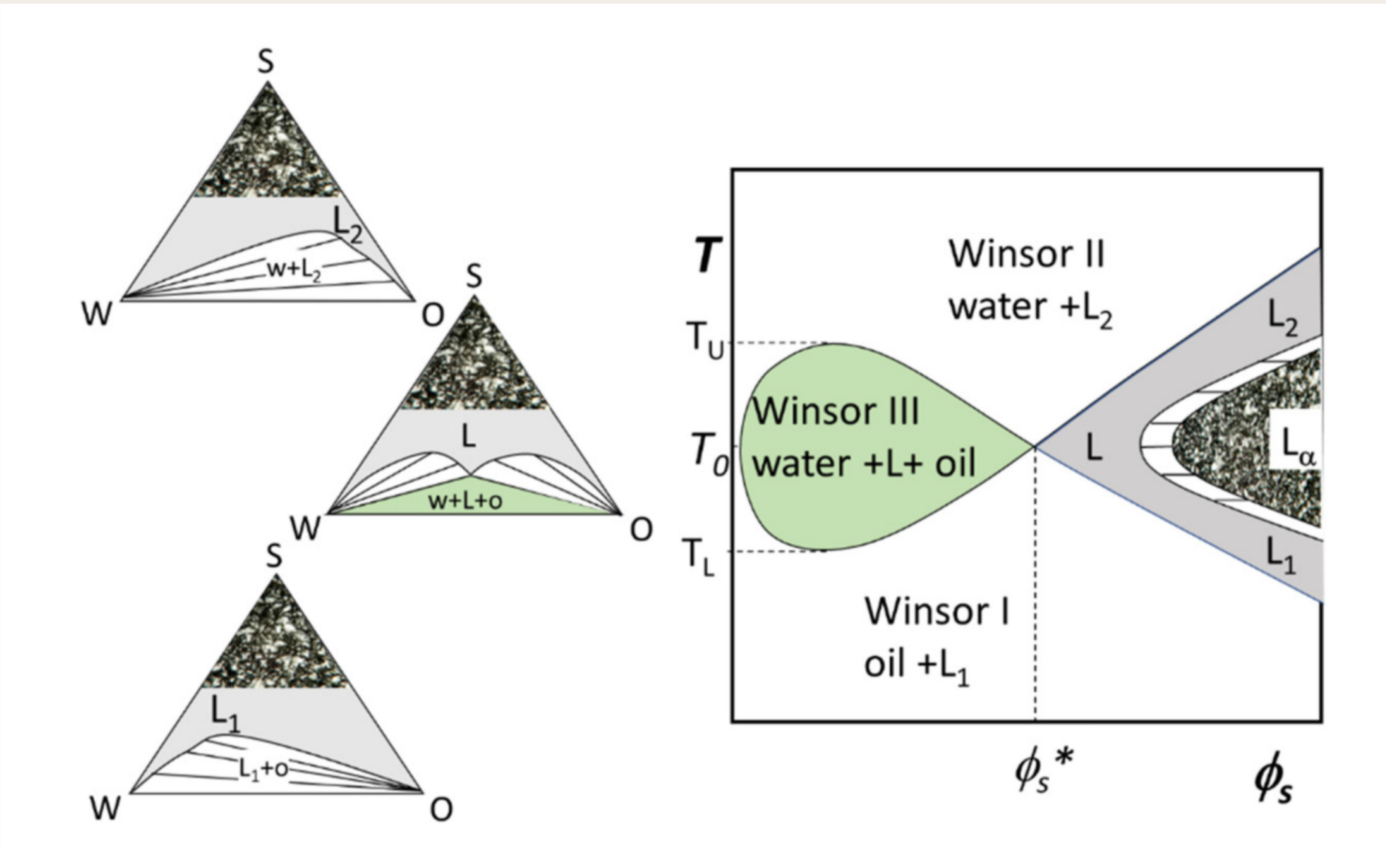


Figure 1: On the left is shown some example ternary phase diagrams, on the right is an example of a fish diagram. The ternary diagram was the first visualization to generate and can be seen in Figure 2. Creating a prism (or tent) diagram allowed for generation of the fish diagram from the HLD-NAC equation, seen in Figure 4. [1]

Purpose

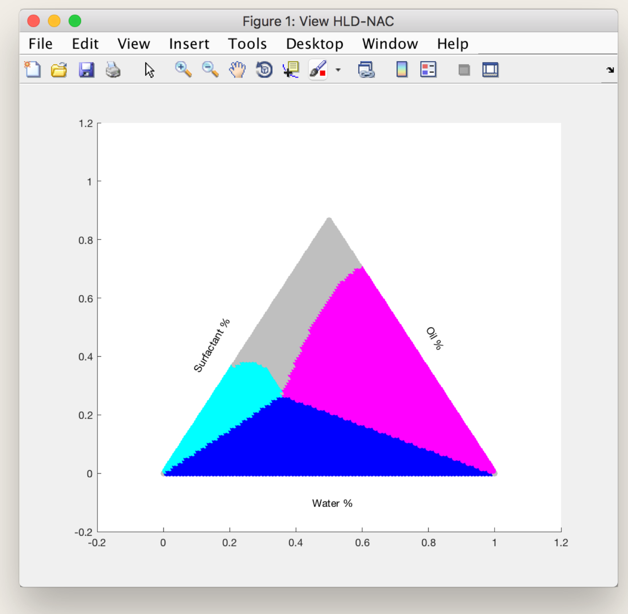
Predicting and understanding solubilization and conductivity behaviors of surfactants has been an area in fuel cell research, and performing experiments can be excessively time consuming. The Hydrophillic-Lipophillic Deviation and Net Average Curvature (HLD-NAC) equations can deliver an acceptable prediction of these behaviors. Our approach to a solution of making this process possible in a reasonable time-frame was to create an interactive simulator which samples the HLD-NAC over a range of input values output to the user as various industry standard views. As the HLD-NAC is still evolving, our implementations have been written to proper software engineering standards so that the implementation can be updated by anyone when the HLD-NAC is improved.

An approximate HLD-NAC equation:

$$HLD = \ln(S) - K \times EACN - \alpha T\,(T - T^{*}) + Cc + f(A)$$

$$H_n = \left|\frac{1}{R_o}\right| - \left|\frac{1}{R_w}\right| = \frac{-HLD}{L} \qquad H_a = {\left(\left|\frac{1}{R_o}\right| + \left|\frac{1}{R_w}\right|\right)}\Big/_{2} \geq \frac{1}{\xi}$$

Which considers aspects of the brine, oil, and surfactant used. The NAC expands and determines the curvature of the microemulsion – which allows for determination of the resulting Winsor type systems.



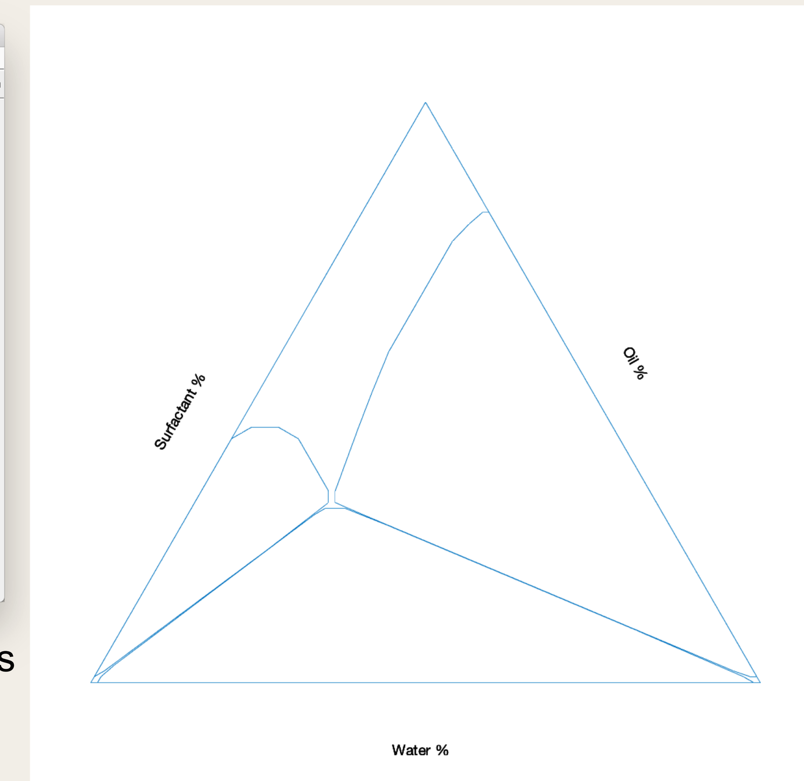


Figure 2: 2D Generated Phase Diagrams
Above: Filled-in scatterplot – allows for fine inspection of the data itself.
Right: A rendition of the same phase diagram for comparison to hand-drawn phase diagrams, or for ease of printing.

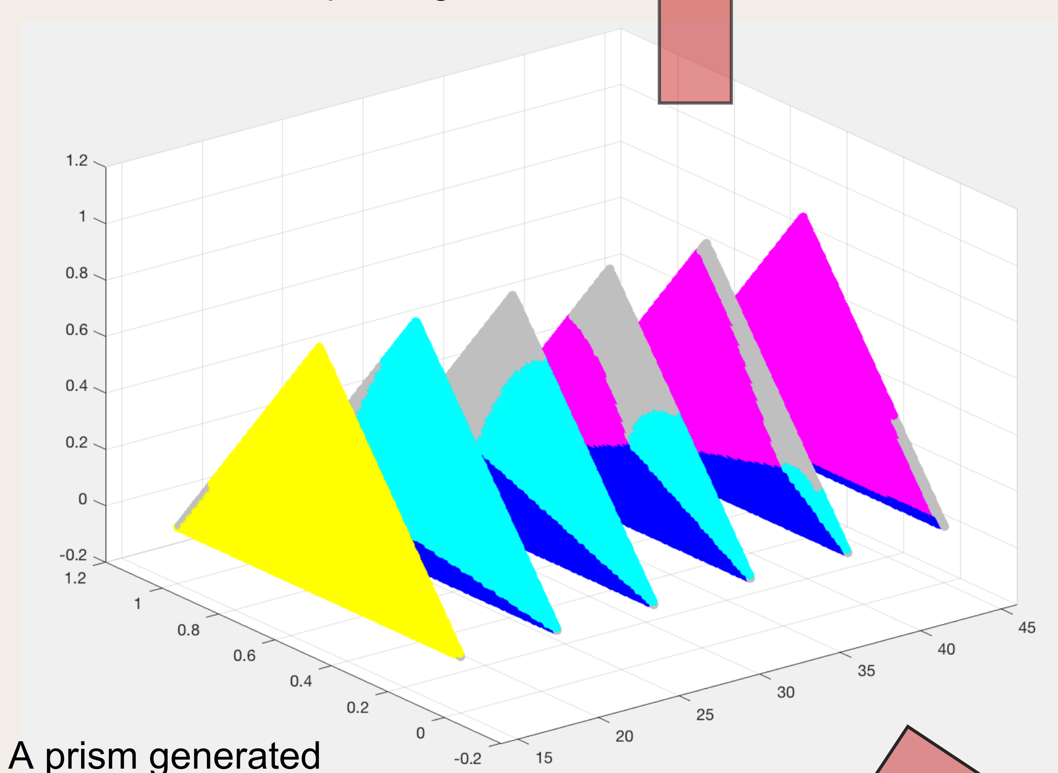


Figure 3: A prism generated as slices, each of which is computed As a 2D ternary diagram. In the current view, the prism is sampled at 1% solubility increments and at 5 ºC increments.

Methods

MATLAB was chosen for creating this project due to:

1) Interactive 2D/3D graphing environment provided
2) Compatibility with future researchers
3) Sufficient elapsed runtime, fast development time

The ultimate task of this project is to render a 4D situation onto a 3D plot, viewed via a 2D screen. First, a 3D cartesian space is generated, which is used to calculate slices of a prism. These slices are used to calculate ternary diagrams via the HLD-NAC/Flash algorithm. If needed, this data is converted to a volume.

Results

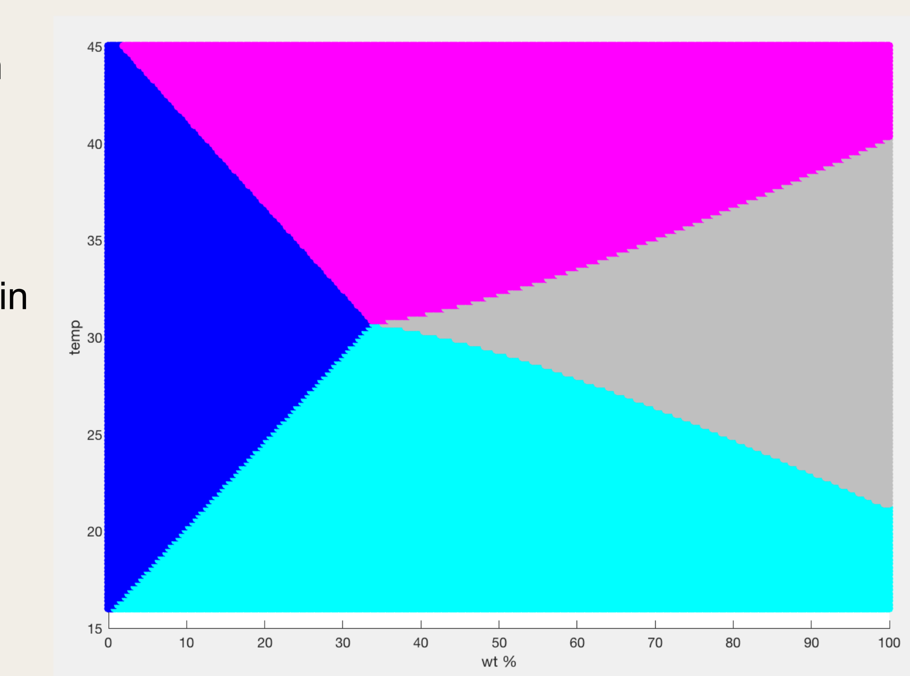
This project provides a user interactive (chosen view can be rotated and viewed alternatively, if wanted) simulator of the HLD-NAC equation. Many circumstances are considered, as well as various inputs dictated by the user.

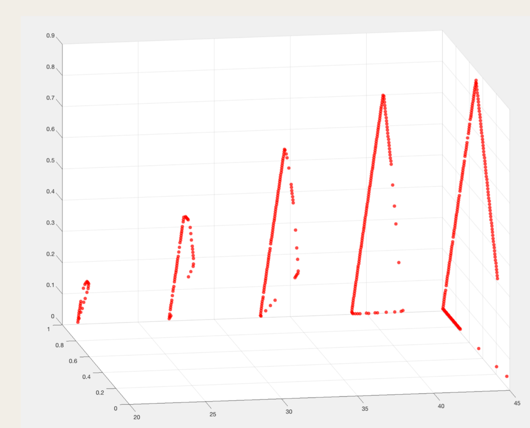
Output views provided include:

1) 2D ternary phase diagrams (filled-in or "sketched")
2) 3D shell, tent, prism, and prism slice renditions
3) Fish diagram and Schinoda diagram
4) Volumes – these can sliced or further analyzed.

All of these views can be improved as the HLD-NAC logic evolves by altering only the relevant code file.

Figure 4: The fish diagram can be extracted from the prism to the left as a lengthwise vertical slice. The axes can vary and have different purposes – in this plot the x-axis is surfactant concentration (%) and the y-axis is temperature (ºC).





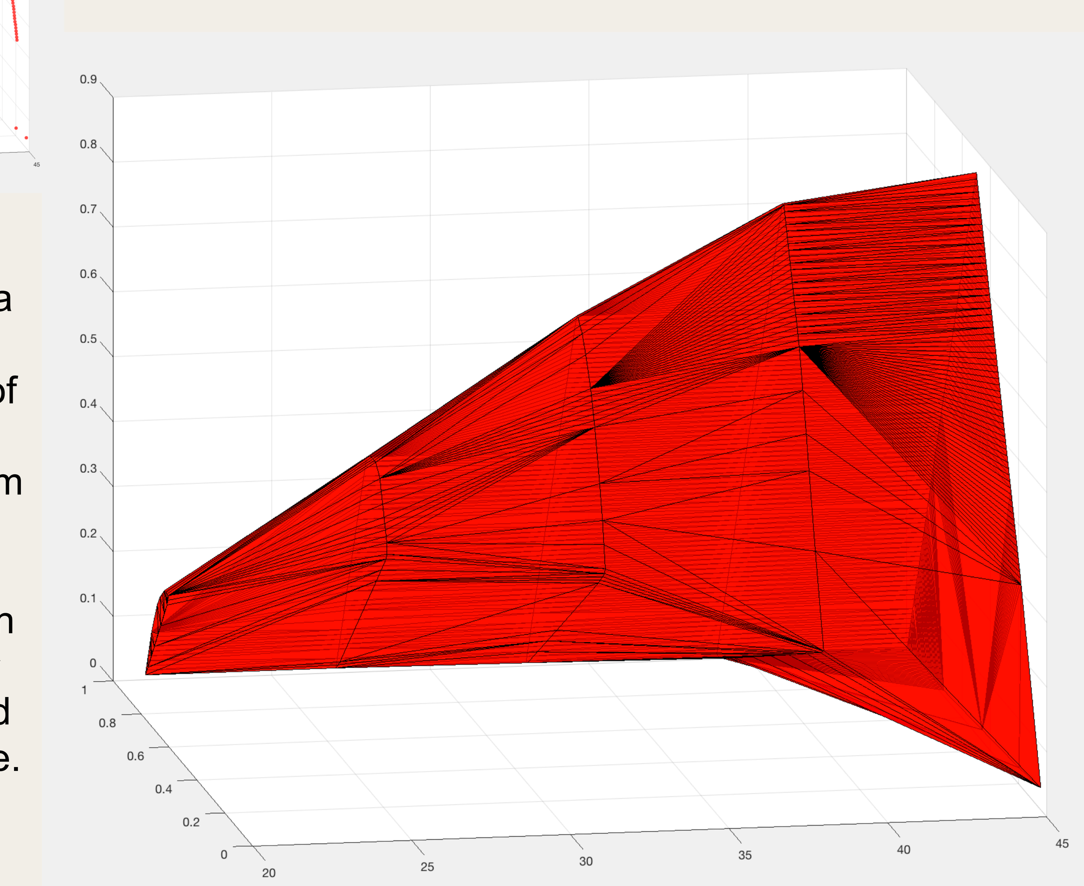


Figure 5: Viewing a single phase type as a volume.
Above: A scatterplot of the sampled data, which is extracted from the prism shown in Figure 3.
Right: The data shown in the scatterplot after being interpolated and converted to a surface.

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1. Tartar, Giuseppe et al. *Microemulsion Microstructure(s): A Tutorial Review*. August 2020. Nanomaterials 1657(10). doi:10.3390/nano10091657

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