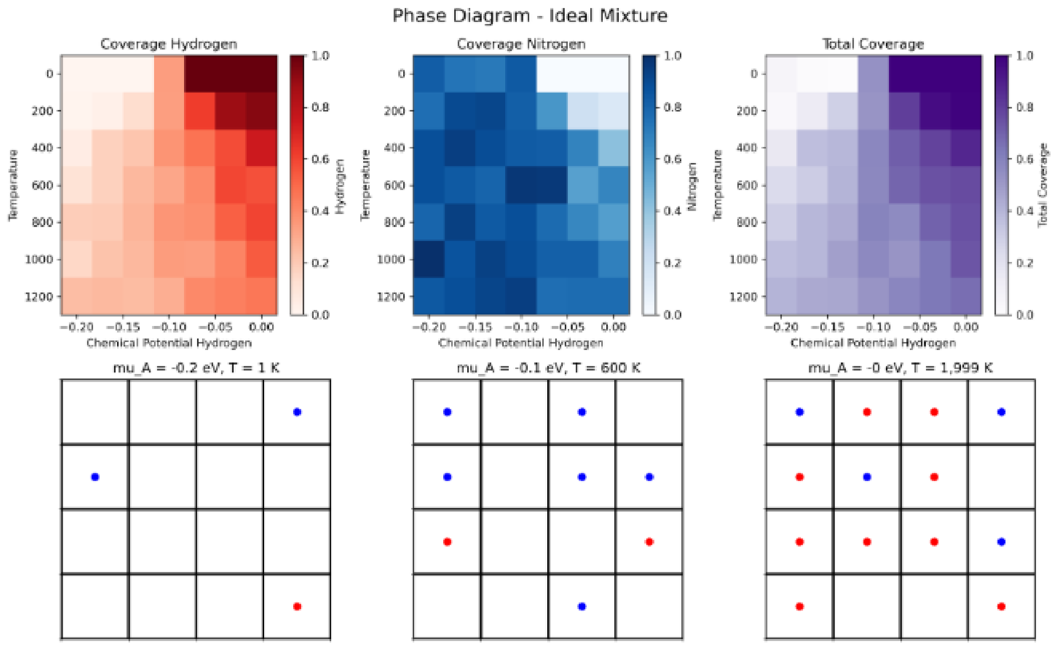
Introduction: The fertilizer industry currently uses the Haber-Bosch process to maximize the efficiency of ammonia production for fertilizers[1]. This process involves mixing hydrogen and nitrogen gases, increasing their pressure and then passing the mixture over a hot iron catalyst at about 723 kelvins. The nitrogen gas is drawn from the atmosphere while the hydrogen is extracted from methane and water. In the report below we will discuss different coverages nitrogen and hydrogen based on temperature differences, varying hydrogen potentials and bond interactions type between the two species; in hopes of finding the most effective interaction type and conditions.

Methods: In this report, we modeled the adsorption of hydrogen and nitrogen on catalytic surfaces under varying experimental conditions, including temperature, hydrogen chemical potential, and types of particle interactions. I utilized a Monte Carlo algorithm to determine whether binding of each particle would take place based on local minimum interaction energy of the neighboring particles. This stochastic approach allowed us to approximate equilibrium surface coverage for different scenarios. The results were visualized using phase diagrams and lattice snapshots, enabling us to analyze trends in hydrogen and nitrogen distribution across the surface under different conditions.

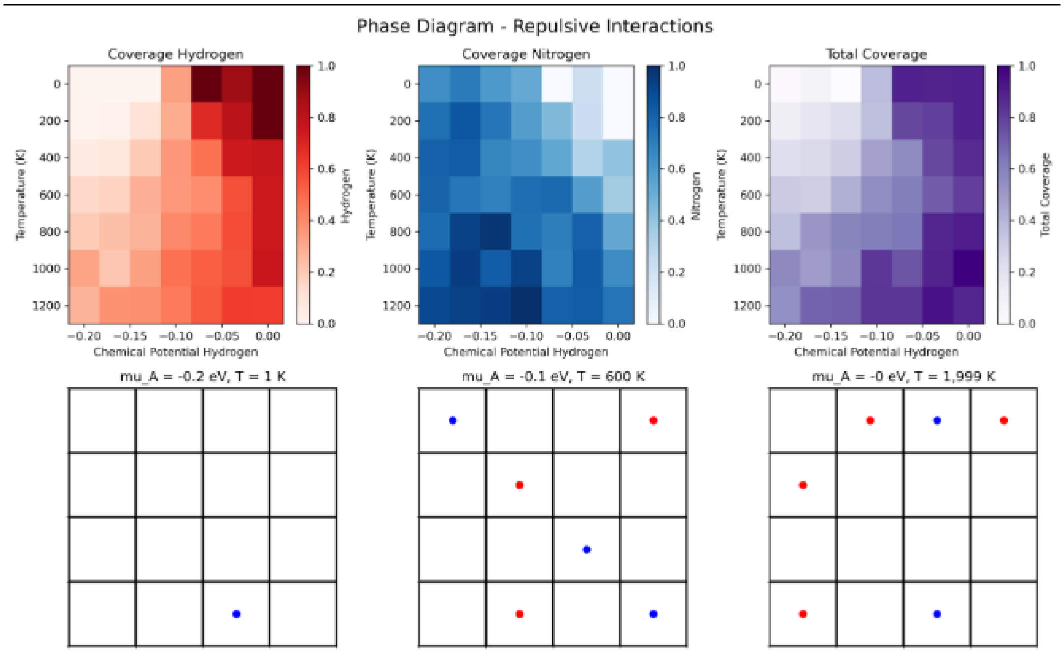
Results: I modeled 5 different interaction types, Ideal gas mixture (Figure 1), Repulsive interactions (Figure 2), Attractive interactions (Figure 3), Immiscible interactions (Figure 4), and finally, likes dissolve unlikes (Figure 5). In each figure the top three plots depict the phase diagrams, the left plot demonstrates the hydrogen bonding to surface with varying potentials energies (hydrogen) and different temperatures starting at 0K on the top and working to 1,200 Kelvin (K) vertically down the graph. The middle plot shows the nitrogen coverage of the surface and finally the top right figure shows the coverage of both species. The bottom plots of each figure demonstrate the lattice (what a small portion of that surface may look like) at three different points. From left to right: chemical potential of hydrogen varies from -0.2 electron volts (eV), -0.1eV, and finally 0eV, in a similar fashion left to right temperature varies from 1K, 600K and finally 1,199K respectively.

Ideal gas: In the ideal gas model there is a clear gradient of increasing coverage of Hydrogen with a corresponding increase of chemical potential. At higher temperatures and higher chemical potentials there is a clear affinity of hydrogen atoms at the surface. The nitrogen is relatively homogeneous throughout with only subtle changes except at temperatures approaching 0 K. The lattice demonstrates similar trends seen throughout the phase diagram with increasing coverage and more hydrogen dominate as the potential increases.



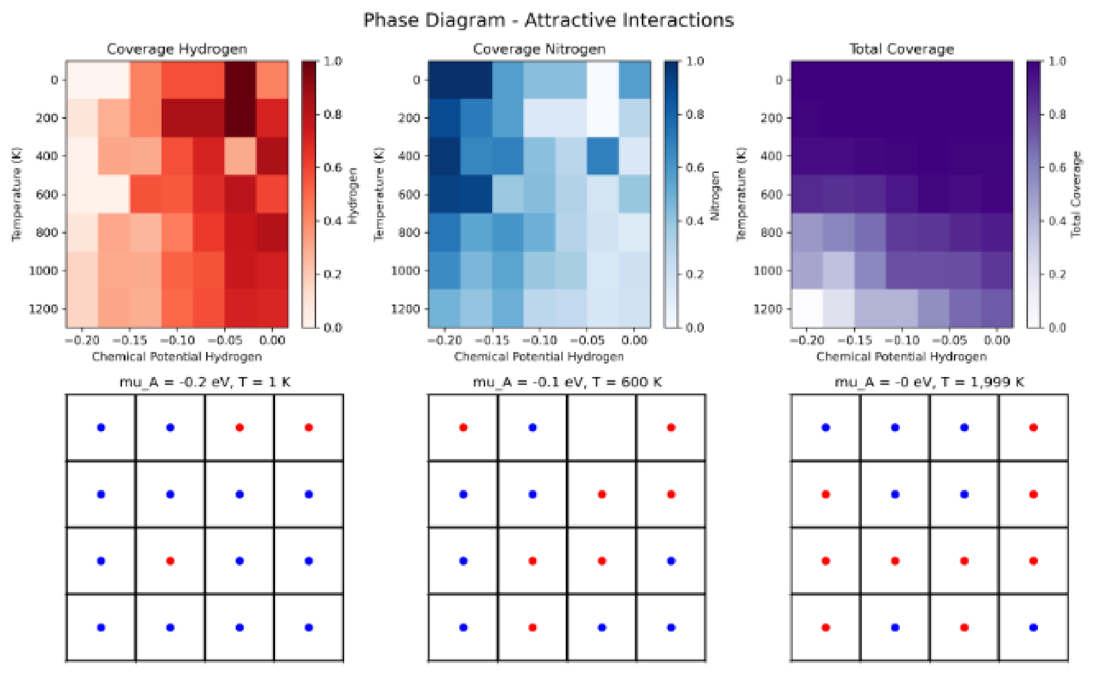
(Figure 1: Phase diagram and coverages up top (Hydrogen, Nitrogen, and total coverage, with lattices below.)

Repulsive interactions: With repulsive interactions there is clear desire for Hydrogen and Nitrogen to be separated from each other. This separation drives many empty spaces in the lattice. There are similar trends to the ideal gas for each individual atom but with the repulsive effects there is a lot of empty space on the surface.



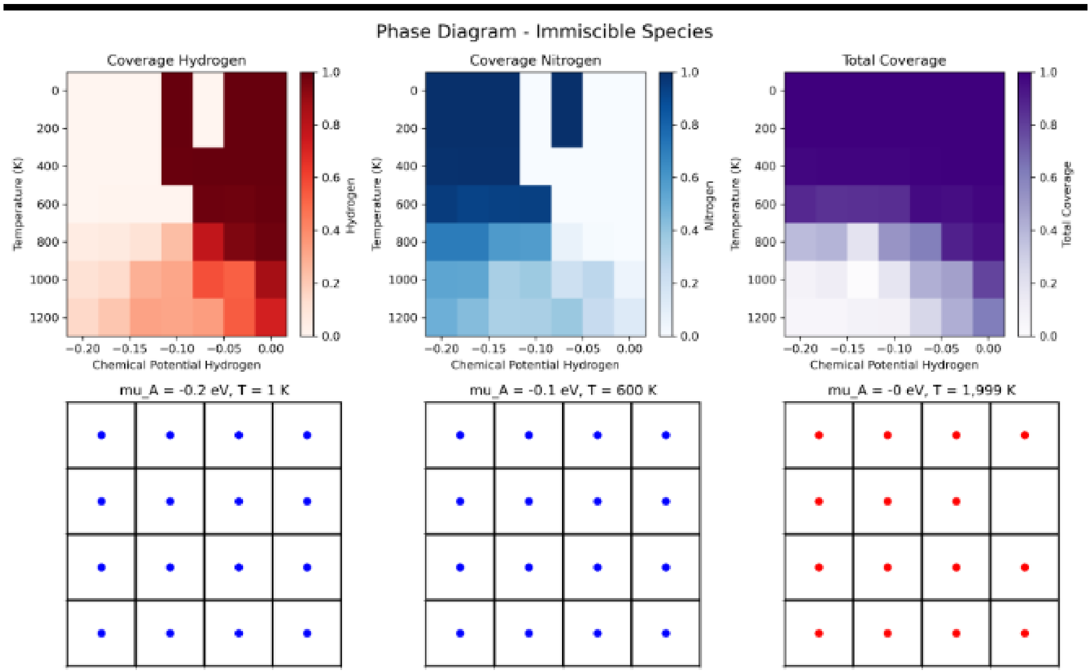
(Figure 2: Phase diagram and coverages up top (Hydrogen, Nitrogen, and total coverage, with lattices below.)

Attractive Interactions: This type of interactions demonstrates a sharper increase in Hydrogen bonding at earlier potential increase; however, it plateaus compared to other phase diagrams. Nitrogen coverage has an inverse relationship to the Hydrogen coverage. The total coverage has reached its maximum below 600 K. It is interesting to note that all lattices are mostly full, however there is room for Nitrogen to dissociate. Overall, this shows high total coverage.



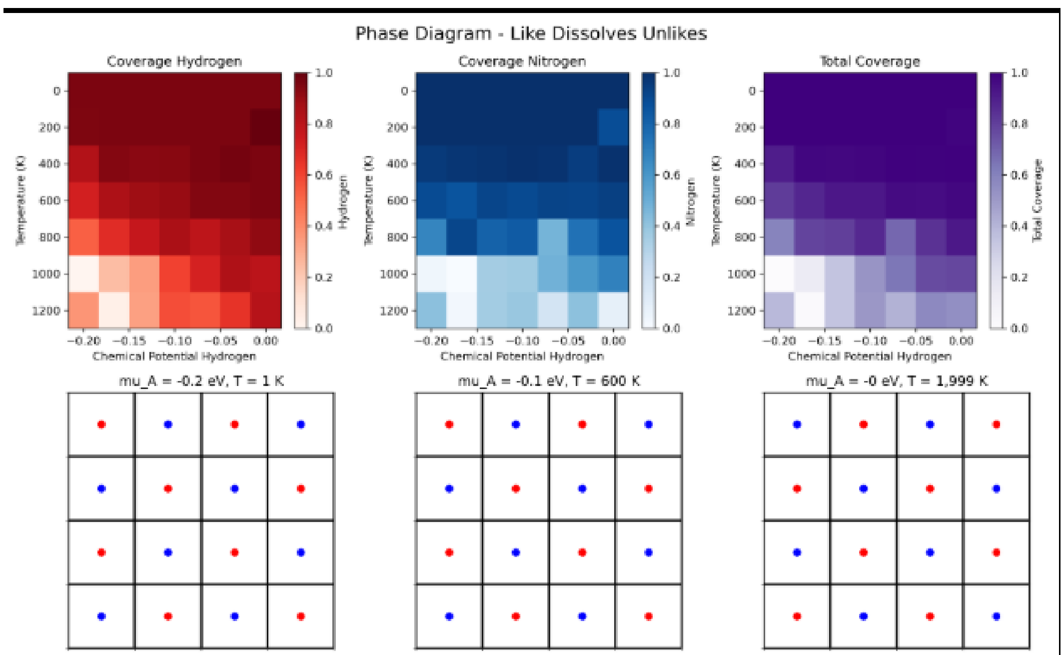
(Figure 3: Phase diagram and coverages up top (Hydrogen, Nitrogen, and total coverage, with lattices below.)

Immiscible: These phase diagrams have very sharp rigid boarders where the Nitrogen and Hydrogen do not prefer to interact. This separation is largely dominated by the chemical potential at lower temperatures but becomes a little blurred at higher temperatures. The coverage of this interaction is high but will largely or only be dominated by one species depending on conditions.



(Figure 4: Phase diagram and coverages up top (Hydrogen, Nitrogen, and total coverage, with lattices below.)

Likes dissolve unlikes: This demonstrates the most unique phase diagram where Hydrogen and Nitrogen want to occupy the same spaces. This leads to a one-to-one ratio of Hydrogen and Nitrogen in a repeated fashion in each of the lattices. Once again there is a loss in coverage at high temperatures and low potentials.



(Figure 5: Phase diagram and coverages up top (Hydrogen, Nitrogen, and total coverage, with lattices below.)

Discussion: To optimize Ammonia production two parameters must be met. First, the total coverage of the surface must be optimized (though it cannot be full at all points to allow dissociation of the Nitrogen species)[1]. Secondly, cost effectiveness must be considered for this process. Fertilizer is necessary for proper farming and food growth; to keep cost low for farmers and the general consumer the cheapest and most efficient method must be utilized. If conditions are expensive and difficult to meet though the production may be optimal, it would not be beneficial upstream. Another important consideration is the boundary conditions of your experiment. Conditions may vary slightly in any apparatus and thus must be considered during production. Using a systematic approach for selecting the optimal condition, I can rule out the ideal and repulsive conditions due to the lack of coverage on the surface. I can rule out the immiscible apparatus because of the competitive bonding that generates a phase separation at the surface; though total coverage is high, this method is just not ideal for generating Ammonia. Both the likes dissolve unlikes, and attractive conditions provide good coverage at reasonable temperatures and potential while allowing both species to co-exist. From this model, the high temperature used in the Haber-Bosch becomes clear as some open spaces at the surface are mandatory for Nitrogen dissociation.

Conclusion: Utilizing this Monte Carlo simulation, I demonstrate that the likes dissolve unlikes model achieves optimal coverage in the simulation but is not physically realistic for bonding on the iron surfaces. The attractive interaction model, while slightly favoring one species at a time, better reflects actual surface chemistry and is more relevant to the Haber-Bosch process. The slight favor for one bonding species over the other for any given parameter could lead to saturation and catalyst poisoning[1]. This model is not without its flaws however, as it does not consider variations in pressure, nor time, and has a relatively small lattice. Increasing the lattice size while tracking time may give better insight into which method is favorable between the attraction interactions and the like dissolves unlikes interaction. If the surface is sufficiently large it would be interesting to determine which model covers the surface quicker.

References:

[1]Wikipedia contributors. (n.d.). *Haber process*. In *Wikipedia*. Retrieved November 17, 2025, from https://en.wikipedia.org/wiki/Haber_process