A Study of Quantum Computing and its Application on Industrial Production of Ammonia

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**Introduction**

A major issue in today’s world is the inefficient production of ammonia. Ammonia is currently an incredibly necessary chemical for the growth of food. The issue that quantum computing may provide a solution to is that the production of ammonia at the level to sustain the global population can not last indefinitely. As the population increases, the need for a more optimized method of production or a system to replace the Haber process used to generate ammonia will be required. Modern methods used in industry to mass-produce the ammonia required in fertilizer use a significant and measurable fraction of the world’s resources. Researchers need to seek new methods of production to combat the expected rise in demand for food growth. A solution currently being pursued is found in nature where bacteria is capable of generating ammonia with much higher efficiency and lower extremity of requirements. Understanding what quantum computers are capable of opens the opportunity to solve nonclassical, quantum problems. The quantum nature of chemical functions that take place on a cellular level makes the ammonia issue a prime candidate for research in quantum computing to provide an answer. This paper focuses on the benefit that quantum computing can provide to assist the optimization of producing ammonia at an industrial level to combat the Haber process of the early 1900s.

**An Overview of Quantum Computing**

To begin to understand the benefit quantum computers can provide to the world, first a general understanding of quantum mechanical principles and their limitations should be gained. Many industries currently hold a stigma against quantum computing as generating algorithms for applications in such industry prove to be a highly difficult task. (Bayerstadler et al., 2021, p. 2). With early quantum computers experiencing small errors occasionally due to their highly specific nature; non-computing fields of study are hesitant to invest in this technology at this time (p. 2). However, the promise of eventual discoveries to answer quantum problems should attract investors in such areas of focus. An example is fields of study which utilize chemistry in some form. Chemical-related occupations and research are expected to be some of the first adopters of quantum computing (Bayerstadler et al., 2021, p. 5). This holds due to the molecular nature of the study of chemistry and its ties to the instability perceived through a classical understanding of quantum probability within individual units of matter at such a minimal scale.

While there are constant improvements to the precision of operations with quantum computing, the issue lies in the quantum instability of small probable variations in the return of measurements from quantum-related operations. There are many aspects of quantum mechanics that are both not fully understood and not fully stable enough to guarantee a certain classical for a quantum probability. A logical principle that can be a major factor in the understanding and application of quantum mechanics is that some quantum attributes that play a major part in how the universe functions do not have classical analogies to bridge the gap in thought process or understanding. This means that researchers in the field of Quantum mechanics and those designing cutting-edge algorithms to apply such mechanics must redefine how they approach these highly complex problems. To reach an understanding of how to solve modern quantum issues (i.e. making the process of ammonia production competitively efficient) those tasked with the work need to define the scope of study to a relativistically new mindset.

**Why is Ammonia Production is Vital**

The focus on ammonia production stems directly from its vital role. The production and utilization of ammonia are ineffective for the recourses it requires. Producing the necessary amount of the product uses up a significant amount of the world's energy and every major global power has some form of focus on its development. Currently, the production of ammonia uses over 1% of the entire world's power consumption (Bayerstadler et al., 2021, p. 5). The driving factor for the continued production of ammonia using the Haber process is the requirement that the population of the world needing sufficient food production to sustain the growing number does not allow for a decrease in the production of ammonia. A continuously growing population demands increased levels of food for its populous, fertilizer to grow said food, ammonia production to make the fertilizer, and, in turn, a new more effective way to generate ammonia (Rafiqul et al., 2005, p. 2487). Thankfully, there is a theoretical solution on the horizon in the form of molecular modeling and research.

**What Benefit Can Quantum Computing Provide Industrial Production**

Since quantum computing can provide solutions to quantum problems and nearly all operations of chemistry are founded in quantum mechanics; a quantum computer theoretically can solve the unknowns of the production of ammonia. Using quantum computing it can be possible to model the NH3 molecule, ammonia, to allow researchers to better understand and predict its exact reactions (Suzuki et al., 2005, p. 360). From this, experts can hope to begin to understand how bacteria are capable of generating ammonia without the requirement of the high heat of industrial production or its other various stages of generation. To accomplish this, the quantum mechanics found in nature should be understood, research in an algorithm to replicate the structure of nature needs to take place, and effort to apply such simulations to the production environment.

Many attributes of observed quantum mechanics play a major role in the way that matter in the universe behaves. Some of the observed properties are expected to play a part in how nature is capable of producing ammonia at such a small scale. This encourages the understanding of the application of fundamentals of the quantum probability of an electron’s location within its classicly measured valence shell, probability of the location of quantum affected particles within their wave function, and, most interestingly, quantum tunneling. Not only does quantum mechanics take a different understanding than classical understandings of physics, when applying theories such as quantum tunneling, but there also exists another level of complexity from the introduction of trajectories from three-dimensional vectors (Yang & Han, 2021). These topics can be studied by experts and applied with a much more complete understanding to produce an actionable outcome. However, in this work, a baseline understanding of the concepts can be presented to understand the implication that quantum computing has on pursuing effective results.

Firstly, in chemistry, the location of electrons within their valence shells and the locations of particles within a factor of their waveform should be addressed. Each particle at the quantum level has its variance in vibration within a constant factor based on highly complex variability (Khrennikov, 2019). This leads to the implication of the need for a way to operate within such a varying and unstable environment. Quantum computers harness the power of quantum probability to provide constants to classical bit values stored in complex numbers known as amplitudes (Brassard et al., 1998). Where a classical machine requires bits to describe a number, quantum machines required amplitudes to describe the combination of classical bits. This allows all states of quantum probability to be described by a single number. Using this strategy, quantum circuits can be designed to use these quantum bits or qbits for computations that classical machines are incapable of processing (1998). The next topic, quantum tunneling, leads to the reasoning for the application of quantum computing to the ammonia problem.

Due to the probabilistic nature of quantum mechanics, there exists a mechanic where particles appear to teleport through objects or barriers known as quantum tunneling. This is a classically confusing event as at first glance, quantum tunneling appears unreasonable. However, through research, we now know there are limitations on quantum tunneling and it is not as bizarre of a process as it may first seem. An example of quantum tunneling is found in the oscillation of inversion of ammonia molecules.

Chart, line chart

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*Figure 1. Likelihood of ammonia molecules inverting through their energy barrier* (Yang & Han, 2021)

Noted above is the observation of an ammonia molecule. Where may seem like the molecule just rotating 180 degrees in the physical space, instead, the molecule has been observed to have its nitrogen atom jump or tunnel through the triangular energy plane that often keeps the atoms spaced apart thanks to their electrons. Given enough kinetic energy, there is a small probability to find the nitrogen atom on the inverted side of the trigonal planar (Yang & Han, 2021). The significant factor of this event is that since this is a quantum event, it is infeasible for a classical computer to model this behavior. However, by harnessing quantum mechanics and quantum computing, there now exists the possibility to better understand why such events happen. If these molecules can be modeled and predicted so can larger structures and systems. From here the cellular bacteria which produce ammonia may be replicable. The hope is that through this study with advanced technology, researchers may be able to decipher what allows nature to generate ammonia with such a higher efficiency than mankind is currently able to produce.

**Conclusion**

We can infer that the applications of quantum technology will be led, at least in their early stages, by tech giants such as (e.g., IBM, Microsoft, Intel, and Google). This being said, the imagination, creativity, and need for quantum solutions to quantum problems in the real world are driving the generations of theoretical ideas to be tested to improve operations of global industry, which in turn, can improve the daily lives of those living on the planet. This is vital as problems such as the sustainment of ammonia production to grow enough food for a rising population will not subside on their own. To find a new way to optimize the production of ammonia, nature's efficient methods of doing so have currently been studied. However, there has been no solution found as of yet. The small scale of operations at the cellular and atomic level can affect how some bacteria can produce ammonia without requiring excessive resources or high levels of heat. By investing in quantum research and studying how the cellular ammonia structure behaves quantumly, there is hope to discover nature’s secret of production. Should this be discovered, we can hope to combat starvation and feed the future populations of a guaranteed increased amount.

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