Expert Insights

Exploring quantum use cases for chemicals and petroleum

Changing how chemicals are designed and petroleum is refined

IBM **Institute for Business Value**

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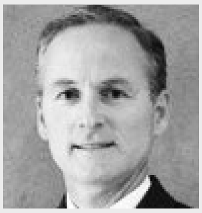

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Doing simulations of chemistry with classical computers, the accuracy of calculations decreases as the complexity of molecular interactions increases.

Talking points

Accelerate discovery
The use of quantum computers by chemicals and petroleum companies has the potential to accelerate the discovery and development of new chemical methods and materials.

Improve margins
Quantum computing may improve the profit margins of chemicals and petroleum businesses by determining optimal combinations of feed-stock routing, refining, and products to market.

Develop quantum advantage
Industry-specific applications that show quantum advantage are likely to be proprietary for the companies that develop them first.

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The promise of quantum computing

Have you ever misplaced your cell phone? You could worry about if it was in your car, at the office, on the floor of the grocery store or you could use a simple app to find its exact location—which is really all you care about, not where it might be. An easy problem to solve for the classical computer in the cloud that your app connects to.

But imagine if you had to track down the effect of an electron moving between states in a quantum world where even the concept of location has become abstract. You would still need to worry about all the states it might have been in, at least in a quantum sense, which is where the power of using a quantum computer starts to impact modelling of chemical systems.

In order to do energy calculations in a quantum mechanical system such as large molecules, calculating all the different parameters including the movement of electrons becomes intractable on conventional computers. As a result, modeling many industrially important molecules becomes increasingly inexact—or simply too time-consuming—to wait for an exact solution.

The chemical industry plays a hand in about 7 percent—or USD 5.7 trillion—of global domestic product, along with approximately 120 million jobs.[1] Developing new chemical products requires expensive and time-consuming lab work. Today, classical simulations of chemistry can help guide lab testing, but the accuracy of calculations decreases as the complexity of molecular interactions increase.

What makes quantum computing more capable of solving these types of problems than classical computers?

The power of quantum

Determining the electronic structure of molecules is imperative to understanding the reactivity of molecule. As molecules increase in size beyond hydrogen (H_2), the mathematical descriptions of molecule that accurately capture electron-electron interactions, nuclear effects, etc. become increasingly complex. In fact, when a full configuration interaction calculation is performed

Quantum chemistry simulations will likely outpace classical solutions once powerful enough quantum computers are built.

classically, the algorithms have exponential scaling. However, due to the nature of quantum algorithms, chemistry calculations have been predicted to scale polynomially, a promising step towards the ability to perform exact calculations on molecules that are currently out of reach.

For example, the simple hydrocarbon, Naphthalene ($C_{10}H_8$), could be modeled with ~116 qubits, but it would require a classical computer with 10^{34} bits to do the same.[2] For perspective, 10^{34} bits is 7.1 billion times the total volume of data predicted to be stored electronically by 2025—perhaps 175 zettabytes.[3]

Quantum computing may change the way chemicals are designed, hydrocarbons are refined, and petroleum reservoirs are located and produced. In the next few years, it may accelerate the go-to-market cycle in the development of new chemical products, refine investment strategies in light of tightening environmental regulations, and optimize complex systems that directly impact profits, such as transportation, refinery, and chemical plant processes.

Eventually, quantum computers may be able to tackle reservoir simulation and seismic imaging. Consequently, quantum computing is expected to fundamentally disrupt the landscape of the chemicals and petroleum industry.

What's the rush?

With the major impact of quantum computing still on the horizon, why is it so important for chemical and petroleum companies to take action now?

It has already been demonstrated that quantum chemistry simulations will likely outpace classical solutions once powerful enough quantum computers are built. Using quantum computers, enterprises may drastically reduce the amount of time it takes to locate oil fields or develop new chemicals. Think about the impact this can have on your company's revenue and risk profile. Now think about the implications if your competitors act and succeed first.

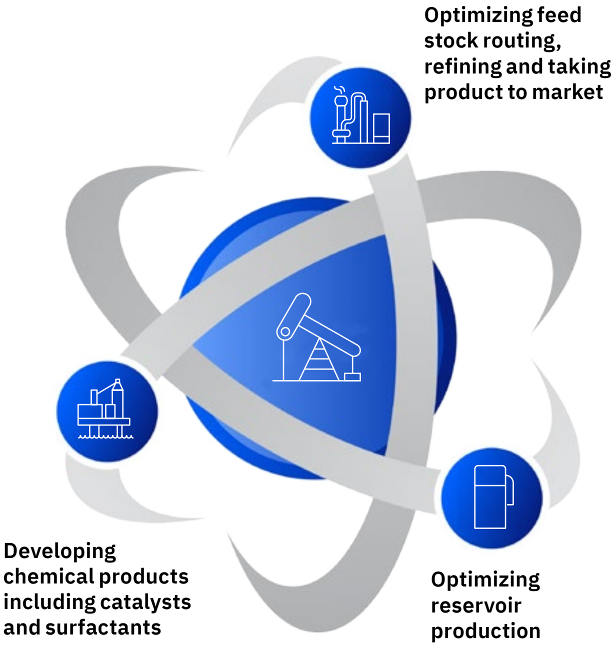
Examining quantum use cases

We have identified three powerful quantum computing use cases already being explored by chemicals and petroleum companies (see Figure 1):

- Developing chemical products, including catalysts and surfactants
- Optimizing feed-stock routing, refining, and taking product to market
- Expanding reservoir production.

Figure 1

Quantum computing use cases in chemicals and petroleum



Source: IBM Institute for Business Value.

Use case 1: Developing chemical products, including catalysts and surfactants

In this use-case scenario, chemical and petroleum companies use quantum computers to accelerate the discovery and development of new chemical methods and materials. Prototype quantum computers, supported by classical computers, are already performing quantum chemistry simulations.

In 2017, a cover story in Nature showed depictions of the small inorganic salts lithium hydride (LiH) and beryllium hydride (BeH_2) modeled on IBM's publicly available quantum computers.[4] Application of these same hybrid methods to challenges in the chemicals and petroleum industry may soon be possible—such as applying insights to new catalysts for emissions reduction or surfactants to improve subsurface recovery. These possibilities, among others, have led some to consider chemistry the "killer app" for quantum computing.[5]

Use case 2: Optimizing feed stock routing, refining and taking product to market

Perhaps surprisingly, similar approaches (using Hamiltonians) employed in molecular modeling can be repurposed to address a wide range of optimization problems, from transportation and supply chain logistics to optimizing investment portfolios.[6]

In this use-case scenario, quantum computing improves the profit margins of chemicals and petroleum businesses by determining optimal combinations of feed-stock routing, refining, and taking product to market. The impact on a refinery can be viewed as the estimated annual loss of business due to octane-giveaway. For 2018, it was USD 11 billion, or 38 percent of the total margin for the refining industry.[7]

Insight: Bits and qubits

In classical computing, the bit is the basic unit of information is used for the representation of two possible states used in coding: 0 or 1.

In contrast, a quantum bit, or "qubit" can hold a superposition of 0 and 1, mathematically described as a linear combination of both states, allowing it to represent more information than a classical bit.

Qubits can be entangled with each other—when qubits are entangled operations on one are coupled to the state of the other. These two properties of qubits, in conjunction with techniques such as amplitude amplification give quantum computers their unique computational power.

Keio Hub Partners: Exploring quantum computing

To explore developing chemistry applications using quantum computing, Japanese chemical companies JSR and Mitsubishi Chemical joined a quantum computing ecosystem—the IBM Q Hub at Keio University in Japan. Both companies expect to leverage the Hub's collaborative partnership of Fortune 500 companies, academic institutions, national research labs and access to 20-qubit and 50-qubit quantum computers to investigate developing quantum computing solutions specific to their businesses.

ExxonMobil: Advancing energy sector application of quantum computing

ExxonMobil is advancing the use of quantum computing in developing next-generation energy and manufacturing technologies, computationally challenging for today's conventional machines. Applications to be explored may include the potential to optimize a country's power grid and the ability to perform more predictive environmental modeling and highly accurate quantum chemistry calculations that enable discovery of new materials for more efficient carbon capture.[10]

Quantum computing ushers in a new age of understanding in subsurface flow dynamics and reservoir simulation.

Use case 3: Expanding reservoir production

In 1856, Henri D'Arcy, a French engineer trying to design water filtration systems for the city of Paris, created a simple experiment by flowing water through a tube filled with sand. His observations led to Darcy's law–which has formed the basis of the entire field of reservoir simulation and production engineering ever since.[8]

However, modern developments in nano-porosity unconventional reservoirs are causing Darcy's law to break down. One outcome is that the global oil hierarchy has been reordered, with the US becoming the world's top energy producer. Quantum computing may usher in a new generation of subsurface understanding and reservoir simulation by allowing the exploration of molecular-scale physics in tight reservoirs.

In unconventional reservoirs, liquid oil flows as if it has a high permeability, similar to a gas, with preferential production of short-chain hydrocarbons and leaving long chains behind. The physics is inconsistent with conventional understanding of subsurface flow dynamics.

In this use-case scenario, quantum computing ushers in a new age of understanding in subsurface flow dynamics and reservoir simulation. Using quantum computers to do molecular scale modelling of the interactions among oil, water, and gas molecules with the surface of rocks helps explain the physics behind the disconnect between Darcy and non-Darcy flow. If so, the benefits would be substantial.

For example, if the number of wells could be reduced by only 10 percent, the net cash flow of the top 32 North American unconventional oil producers would shift from a net loss of USD 1 billion (January to September 2018) to a positive cash flow of USD 8 billion (based on an estimate of USD 6 million per well).[9]

Action guide

Exploring quantum use cases for chemicals and petroleum

The chemicals and petroleum industry is likely to benefit significantly from quantum computing. However, industry-specific applications that show quantum advantage are likely to be proprietary for the companies that develop them first. Embracing quantum computing as an emerging technology necessitates a different way of thinking, a new and highly sought-after set of skills, hybrid IT architectures, and novel corporate strategies. Imagine some of the capabilities and benefits described above in the hands of your top competitors. That's why the time to get started with quantum computing is now—while standards, strategies, use cases, and ecosystems are still being developed.

1. Explore applications

Challenge quantum champions in your organization to experiment with actual quantum computers and explore the potential applications of quantum computing for your specific business. This can already be done on the cloud.[11] To help focus on your highest-value problems, have your quantum champions report to a quantum steering committee that includes line-of-business executives and market strategists.

2. Prioritize use cases

Understand and prioritize quantum computing use cases specific to your industry according to their potential for attaining business advantage—given your organization's business strategy, associated customer value propositions, and future growth plans. Keep an eye on progress in quantum application development to stay in the vanguard of which use cases might be commercialized sooner rather than later.

3. Leverage an ecosystem

Consider partnering with a world-class leader in quantum and an ecosystem of like-minded research labs and academic institutions, quantum technology providers, quantum application developers and coders, and start-ups with supporting technologies.[12] Include organizations with similar challenges to gain immediate access to an entire quantum computing stack capable of developing and running quantum algorithms specific to your business needs. Look for breakthroughs in quantum technology that might necessitate a change in ecosystem partners.

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