Quantum Computing: An Emerging Tool for Chemical Engineers

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Quantum computers received attention in 1982 when physicist Richard Feynman gave a talk explaining that classical computers could not process calculations that describe quantum phenomena, and a quantum computing method was needed for these complex problems *(1)*. In the mid-1990s, Peter Shor developed a groundbreaking algorithm that proved a quantum computer can calculate the prime factors of a large number exponentially faster than classical computers, demonstrating the power of this new technology. Fast forward to today, an increasing number of companies, startups, and academic research laboratories now rely on quantum computing to accelerate the process of developing novel technologies.

It is predicted the quantum computing market will grow rapidly in the next 10 years, driven by its use in pharmaceutical, chemical, and biological applications. Some large and complex problems that engineers in these industries must tackle require a massive amount of computational power to solve, which classical computing is not able to provide. Quantum computing technology has been shown to be especially useful when solving problems involving chemistry, artificial intelligence, simulation tasks, complex correlations among interconnected elements, and large sets of data outside the scaling limits of classical computers. The unique way quantum computers use probabilities and entanglement make them a particularly useful tool for many optimization problems.

Quantum computers store information in qubits, *i.e.,* quantum bits. Unlike classical computing bits that exist as either a 0 or 1, qubits exist in superpositions of 0 and 1, and use entanglement and interference to solve computations with a large number of states. It is estimated that a quantum computer with only a few hundred qubits would be able to perform more calculations than there are atoms in the universe. However, such a computer is yet to be built due to technological limitations — the best quantum computers today have around 50 qubits *(2)*.

Quantum computing tools have several relevant applications in environmental engineering. For example, these tools can be used to study the reactivity of catalysts. Currently, the chemical catalysts used in fertilizer production account for 2% of global carbon dioxide emissions. Engineers could use quantum computing to develop more sustainable catalysts with a lower environmental impact. Additionally, quantum computing can help engineers uncover catalysts for carbon capture that are cheaper and more efficient than current options, which could help to accelerate the widespread adoption of this technology.

Biomedical engineers have shown that quantum computing can have various healthcare applications, such as the development of improved therapies for cancer treatment. For instance, quantum computers can analyze thousands of variables to develop radiation plans that target cancer cells at the ideal dose and target, minimizing damage to healthy cells. Quantum computing has been used to interpret diagnostic images with the help of machine learning tools. In addition, quantum computing tools can reduce the time and improve results of *in silico* drug discovery.

Prominent companies are already recognizing the potential of quantum computing. For example, Google built a quantum computer that could simulate a simple chemical reaction. ExxonMobil is advancing quantum computing technologies to optimize power grids, perform more-predictive environmental modeling, and develop new materials for carbon capture. Japanese chemical companies JSR and Mitsubishi Chemical joined the IBM Q Hub at Keio Univ. to leverage access to 20- and 50-qubit quantum computers to investigate challenges unique to their businesses. Monetary support from private equity and venture capital has birthed startups that specialize in using quantum technology for a variety of applications.

Several gaps and challenges remain before quantum computing can be broadly used in the chemical and biological engineering communities. However, the pace of development is rapid, and we are likely to start seeing the broad adoption of this technology within the next few years. Quantum computing will need to be incoporated into chemical and biological engineering curricula to prepare students to adapt and leverage these developments in their future careers.

AIChE, along with the Technical Univ. of Denmark and Knowledge Hub Zealand, will host the Quantum Computing Applications in Chemical and Biochemical Engineering Workshop on Oct. 21–23, 2021 in Copenhagen, Denmark (www.aiche.org/qc). The workshop will bring together scientists and engineers from academia and industry at all career stages to showcase advances in an emerging and rapidly growing field. Session topics include advanced quantum computing applications, quantum computing in the startup space, and the future of the field. Please contact Nahida Alam at nahia@aiche.org for any questions. CEP

1. **Gamble, S.,** "Quantum Computing: What It Is, Why We Want It, and How We're Trying to Get It," in "Frontiers of Engineering: Reports on Leading-Edge Engineering from the 2018 Symposium," National Academies Press, Washington, DC (Jan. 28, 2019).
2. **Knight, W.,** "Serious Quantum Computers Are Here. What Are We Going To Do With Them?" *MIT Technology Review,* www.technologyreview.com/2018/02/21/145300/serious-quantum-computers-are-finally-here-what-are-we-going-to-do-with-them (Feb. 2018).