Chapter 6
Harnessing Quantum Computers for Efficient Optimization in Chemical Engineering

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ABSTRACT

Quantum computing (QC) has made it possible for optimization and machine learning to get better. These improvements could have big effects on many areas, like medicine, technology, communication, and finance. There will probably soon be a huge rise in the use of QC in the chemistry, pharmaceutical, and bio-molecular fields. Improvements in quantum hardware and software have sped up the process of putting QC into action. It is very important to find real-life chemical engineering problems that cutting-edge quantum methods could help solve, no matter if they are used in computers today or in the future. The authors go over some basic QC ideas while also talking about the problems with current quantum computers. There is also an outline of quantum algorithms that, when used with current quantum computers, could help chemical engineers with machine learning and optimization. There are also plans for future quantum devices because this research looks into linked uses that could use quantum algorithms run on them.

DOI: 10.4018/979-8-3693-4001-1.ch006

INTRODUCTION

De Cao 2018 As new technologies like machine learning and quantum computing become more common, chemical engineering is just one field that could be completely changed. By combining machine learning and quantum computation, it might be possible to make difficult jobs in this area much easier to do. This introduction piece will talk about the possible uses and benefits of combining machine learning and quantum computation to help solve optimisation problems in chemical engineering. Using quantum physics principles, computers that work in this way might be able to solve certain types of problems ten times faster than classical computers. Quantum bits, or qubits, can be in more than two states at the same time, while classical bits can only be in two states, 0 and 1. This means that quantum bits can be used for parallel processing and exponential computing.

Flam-Shepherd 2020 Methods that use machine learning are becoming more popular in chemical engineering because they can look at very large datasets, guess complicated events, and make processes run more smoothly. It has been shown that machine learning algorithms are very helpful in fixing many business problems, like process optimisation and molecular modelling. The coming together of quantum computing and machine learning has opened up new ways to solve efficiency problems that can't be solved with traditional methods. In contrast to traditional optimisation methods, quantum machine learning algorithms have a big edge over them because they can quickly traverse very large solution spaces by using quantum entanglement and parallelism.

P.S. Ranjit 2014 The area where this can be used is chemical engineering, where efficiency is essential for creating high-yield, low-cost processes. Molecular models, chemical reactions, material design, and supply chain management are just a few of the areas where quantum machine learning could be very useful. Chemical engineers can speed up innovation and come up with new solutions by using quantum optimisation methods. There are some good things about combining machine learning and quantum computation in chemical engineering, but there are also a lot of problems, such as hardware limitations, the need to build new algorithms, and data that doesn't work with each other. Interdisciplinary collaboration and ongoing study projects are necessary to find solutions to these problems. Still, as quantum computing and machine learning get better, it becomes more likely that chemical engineering optimisation will lead to game-changing ideas.

DeGroat 2024 Finally, the coming together of machine learning and quantum computation has given us a new way to look at problems in chemical engineering that need to be optimised. With the help of different machine learning techniques and the huge computing power of quantum systems, engineers and scientists may be able to open up new opportunities in the chemical industry that are marked by greater sustainability, efficiency, and creativity. As we learn more about this interesting field, we expect it to have a big effect on how chemical engineering is optimised.

RELATED WORK

Brown, 2019, Krenn, 2020 One type of computer is a quantum computer, which uses quantum mechanical events to do calculations. This way of doing calculations is called quantum computing (QC). Quantum computing could give huge amounts of computing power, which would lead to revolutionary progress in many areas of science and technology. With the development of quantum computers using ML and the proof that quantum computers are better at some tasks, there is a lot of interest in quantum