Korean J. Chem. Eng., 39(4), 811-820 (2022)
DOI: 10.1007/s11814-021-1027-6
pISSN: 0256-1115
eISSN: 1975-7220

INVITED REVIEW PAPER

New frontiers of quantum computing in chemical engineering

Akshay Ajagekar and Fengqi You†

Cornell University, Ithaca, New York 14853, USA
(*Received 5 October 2021 • Revised 10 November 2021 • Accepted 29 November 2021*)

Abstract−Quantum computing (QC) has the potential to strongly impact various sectors like finance, healthcare, communication, and technology by driving innovation across optimization and machine learning. Applications of QC in chemical, pharmaceutical, and biomolecular industries are also predicted to grow rapidly in the near future. Advancements in quantum hardware and algorithms have helped accelerate the widespread adoption of QC. Yet, despite the progress, several research gaps and challenges need to be addressed before leveraging QC for chemical engineering applications. Quantum computers offer higher computational power due to the exploitation of their quantum mechanical properties. However, not all computationally intractable problems can benefit from QC's computational abilities. Achieving speedups over classical computing with quantum algorithms implemented on current quantum devices is possible for a few specific tasks. It is imperative to identify chemical engineering problems of practical relevance that may benefit from novel quantum techniques either with current quantum computers or of the future. Here, we present an introduction to basic concepts of QC while identifying the limitations of current quantum computers. A review of quantum algorithms that may benefit optimization and machine learning in chemical engineering with current quantum computers is also provided. This work also sets expectations for quantum devices of the future by exploring similar applications that may benefit from quantum algorithms implemented on such devices.

Keywords: Quantum Computing, Machine Learning, Deep Learning, Optimization, Artificial Intelligence

INTRODUCTION

Quantum computing (QC) refers to calculations performed by harnessing quantum mechanical phenomena, and devices that realize the same are called quantum computers. QC has the potential to support transformative advances in several fields of science and engineering due to its potentially enormous computational power [1]. Owing to the realization of quantum computers through technological advancements [2] and claims of quantum supremacy for certain problems [3], QC has acquired significant research interest and capital investment in its physical implementation. The widespread real-world implications of achieving substantial speedups with quantum algorithms [4] have further contributed to the progress and development of QC. Many initiatives are underway to revolutionalize the fields of communication [5], finance [6], and artificial intelligence [7] with emerging technologies like QC. The advantages offered by QC's computational abilities originate from innovative use of quantum algorithms and devices to handle specific tasks, and in turn, not limit its applicability to these areas. There are relevant chemical engineering applications that can also be efficiently tackled through careful deliberation over adopting appropriate QC technologies.

Early motivation for developing a quantum computer started with simulating quantum mechanical phenomena in the 1980s [8,9]. The advent of quantum algorithms that demonstrated better computational efficiency over classical algorithms further accelerated this cause. For example, the need for efficient execution of Shor's algorithm for large integer factorization has been a key contributor to the advancement of QC [10]. Recently, research efforts have been directed towards identifying problems that can be solved easily with a quantum computer but remain unsolvable [11] or require prohibitively large computational time by the fastest classical computer [3]. Quantum computers are expected to surpass the computational performance of classical computers for such problems since their computational power grows exponentially with the number of qubits. Qubits are the basic unit of information in QC that possess quantum mechanical properties, which sets quantum computers apart from classical computers. A peek into widespread impact on areas ranging from finance to defense has further promoted the research and development of QC devices focusing on increasing their scalability while mitigating associated errors in operation. In addition to high-end quantum hardware, software that enables their efficient control for building quantum algorithms to address problems of practical relevance is equally important. Various quantum software, including tools and libraries to execute quantum programs, as well as quantum simulators that allow for validating such programs, can help exploit QC's potential for real-world applications [12].

Chemical engineering encompasses a broad range of problems in science and engineering, including, but not limited to, reaction engineering, transport phenomena, unit operations, the study of biochemical processes, energy systems optimization, materials design, and green chemistry [13]. Modeling, design, and optimization of complex systems is integral to the development of safe and adaptable techniques for applications in these areas. Optimization in chemical engineering is required for efficient resource utilization, lowering the capital and operating costs, reducing the environmen-

†To whom correspondence should be addressed.
E-mail: fengqi.you@cornell.edu

tal footprint of chemical processes, as well as the design of materials with desired properties [14,15]. Machine learning has also had a significant impact on chemical engineering applications [16] with the replacement of traditional approaches with data-driven techniques for improved flexibility and accuracy [17]. Classical optimization and machine learning techniques may not scale with large-scale applications either due to the intractability of solution approaches or inefficient computational operations. QC techniques could potentially help speed up certain aspects of optimization and learning tasks in chemical engineering through high-performance information processing offered by quantum devices.

Even though quantum circuits are able to simulate any classical circuit [1], a computational advantage with quantum computers can be expressed only for certain tasks. Additionally, the technological limitations of current quantum devices curb the fidelity of computations performed with the quantum algorithms. Quantum systems that cannot be simulated by brute force using even the most powerful digital computer can be referred to as noisy intermediate-scale quantum (NISQ) devices with their computational power limited by noise or imperfect hardware [18]. Fault-tolerant QC indicates the quantum system's ability to detect and mitigate errors associated with noisy qubits. It is utmost important to identify problems in chemical engineering that may benefit from quantum techniques implemented on today's quantum computers without compromising the quality of results. There have already been a few attempts to use quantum techniques for several chemical engineering-related applications, like quantum chemistry simulations [19], process scheduling [20], and supply chain logistics [21,22]. In this work, we introduce readers, specifically researchers, and practitioners in chemical engineering, to the groundbreaking technology of QC while also creating awareness of its shortcomings. We begin by discussing the primary components of any quantum computer in Section 2, followed by the specific models of computation in QC. Section 3 provides an overview of the current status of quantum computers and challenges faced by today's quantum devices, along with their characterization in terms of errors and fidelities. We further discuss the current and near-future implications of QC on optimization and machine learning for chemical engineering applications in Section 4. The impact of realizing quantum devices that match expectations outlined in Section 3 on similar applications is briefly provided in Section 5. Conclusions are drawn in Section 6.

QUANTUM COMPUTERS

In this section, we introduce the underlying building blocks of quantum computers, their types, and the corresponding operations. A quantum computer is comprised of three primary components: the quantum memory, the quantum processing unit (QPU), and an input/output module that communicates information to and from the QPU [23]. Quantum memory, which is essential for the development of quantum devices, stores quantum states for later retrieval and manipulation as quantum bits. A quantum bit, or qubit, is the fundamental unit of QC and is analogous to the bit in classical computing. The quantum state of a qubit can be represented by a linear combination of its basis states, *zero* and *one*, where the multiplier constants indicate the probability amplitudes. These probability amplitudes encode not only the probability of measurement outcomes but also the phase relative to the basis states [1]. This means that a qubit state is in a superposition of the basis states, and the probability of that qubit collapsing into either of its basis states is dictated by the probability amplitudes.

Additionally, two or more qubits can form strong correlations between their individually random behaviors and is termed as entanglement [1]. Quantum entanglement allows us to infer the state of one qubit by measuring the other. The quantum mechanical properties of superposition and entanglement are inherent to qubits and are responsible for the exponential growth in computational power by adding more qubits, in contrast to the linear growth in classical computing power obtained by adding more bits. The QPU is a computational unit that allows for manipulating states of the qubits by performing operations guided by quantum mechanical principles to perform a particular task [24]. A quantum system consisting of multiple qubits is also referred to as a quantum register. An interconnected network of qubits is placed within the QPU, where the physical connections dictate the allowable qubit operations. Upon measurements of the quantum state, the resulting bit string is also stored in a classical register within the QPU. Input to the QPU refers to the initialization of qubits in the QPU to the desired state, while either *zero* or *one* obtained after measuring a qubit state is the obtained output. Computations performed within the QPU by performing operations on the qubits are defined by the specific quantum computational model. Details for the realization and operation of two widely adopted models of quantum computation are provided in the following subsections.

1. Quantum Circuit Model

A popular and well-developed model for quantum computation is the quantum circuit model that was proposed for universal QC and is also referred to as the Deutsch model [25]. Computation in the quantum circuit model is carried out by a sequence of quantum gates. Quantum gates are the key components of a quantum circuit and are analogous to the classical logic gates in classical digital circuits. Contrary to most classical logic gates, the quantum gates are reversible due to the unitary nature of quantum mechanics [1], meaning that the gate's inputs can be reconstructed from the gate's outputs by applying an appropriate unitary transformation. Theoretically, this means that quantum gates do not lose information during the transition of the qubit from one quantum state to another. They are represented by unitary matrices and operate through matrix multiplication with the vector space of a qubit system. A quantum circuit includes an ordered sequence of quantum logic gates that operate on multi-qubit registers coherently. A diagram for one such quantum circuit is shown in Fig. 1.

Each wire in the quantum circuit diagram represents the quantum state of that particular qubit. The quantum state of a qubit refers to the complex probability amplitudes corresponding to the basis states *zero* and *one*. Quantum gates are applied chronologically from left to right of the circuit diagram, as shown in Fig. 1, meaning unitary transformations dictated by the particular gate are sequentially applied to the qubit state. As seen in the quantum circuit, some quantum gates like Hadamard (H), Pauli-Z (Z), and T-gate (T) operate on single qubits, while gates like controlled-NOT ($\oplus$) transform

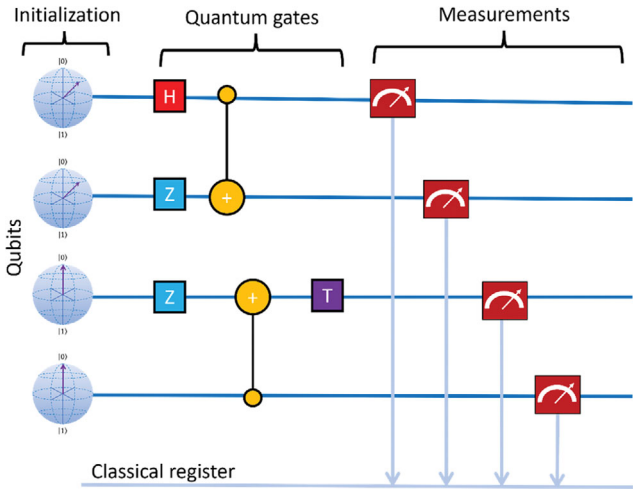

Fig. 1. Gate model quantum computer with unitary gates as qubit operators.

the state of two qubits simultaneously. Apart from gates, a quantum circuit also consists of measurement operators and initialization steps. The initialization of a quantum state can be performed by applying single-qubit gates to the qubit basis state. Additionally, the measurement operator in the circuit measures the qubit register and outputs classical information, which is further stored in the classical register within the QPU. It should also be noted that the operation of multi-qubit gates is governed by the connectivity between the associated qubits on the QPU. Quantum algorithms can generally be represented as quantum circuits. These algorithms consist of three basic steps mentioned above: encoding data into a set of qubit states, sequential application of quantum gates to this set of qubit states, and measurements of one or more qubits that yield classically interpretable information [26].

2. Adiabatic Quantum Computing

An alternative to the more familiar quantum circuit model of computation is adiabatic quantum computing (AQC). Unlike the quantum circuit model that resembles classical digital computing, AQC is analog [27]. AQC is built upon the quantum adiabatic theorem, which dictates that a quantum system in its ground state remains in a ground state, provided that the evolution of the state is slow. In the context of quantum mechanics, adiabatic refers to a slow process that is almost always at equilibrium [28]. Since computation in AQC is a reversible process that is carried out very slowly, the term "adiabatic" is used to describe the mode of computation. In AQC, computation proceeds by continuous-time evolution of a quantum state from a known initial state to a final state under adiabatic conditions [29]. The adiabatic evolution of a quantum system involving four qubits is shown in Fig. 2. AQC was introduced as an approach for solving optimization problems termed "adiabatic quantum optimization" [30] but has since evolved into a universal model of computation that employs the quantum mechanical principles manifested in quantum physical systems. The universality of AQC has been established by showing that it is computationally equivalent to the circuit model of quantum computation [31].

A multi-qubit quantum dynamical system that evolves over time according to forces acting on it is shown in Fig. 2. Such forces can be characterized by a time-dependent Hamiltonian H. At time t=0, an initial well-defined Hamiltonian is chosen such that the ground state can be prepared easily. The system then slowly evolves towards problem Hamiltonian by introducing qubit biases h and couplings J between the qubits achieved with the application of external magnetic flux. The intensity of such magnetic fields is programmatically controlled through analog signals within the QPU. The adiabatic evolution from a known initial state to the final ground state of the problem Hamiltonian after total evolution time t= τ, as shown in Fig. 2, represents the AQC model of quantum computation. The realization of AQC using quantum systems poses a major challenge concerning their control stemming from the non-idealities present in the system. Due to the technological limitations in maintaining adiabatic conditions, a relaxation of the adiabatic con-

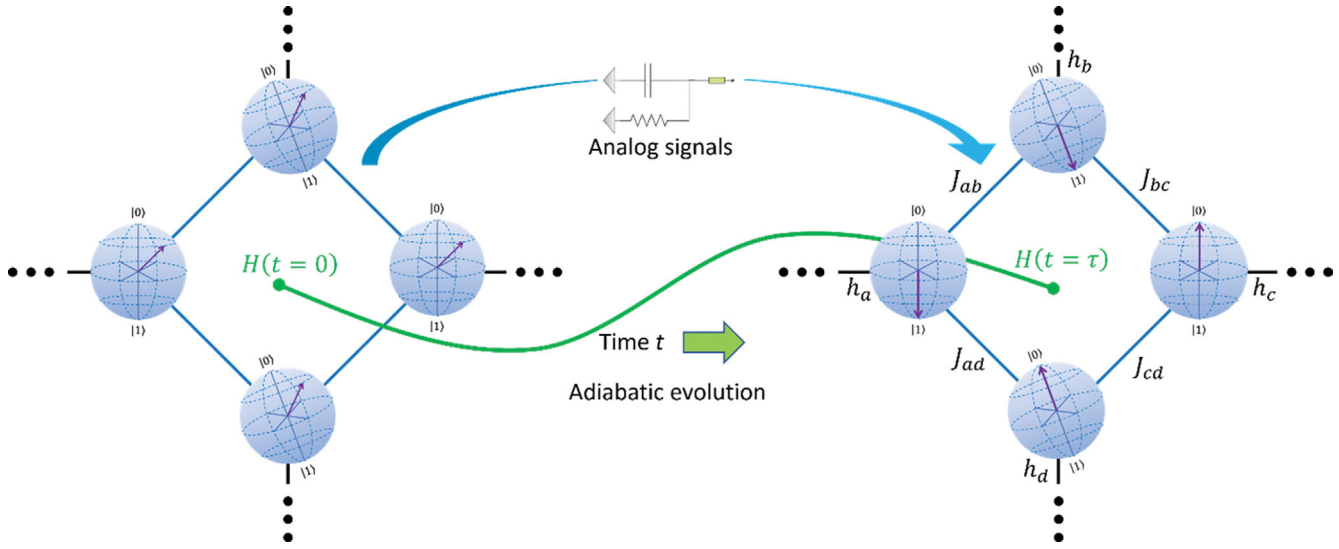

Fig. 2. Evolution of state in AQC devices from the ground state of initial Hamiltonian to that of problem Hamiltonian.

ditions can be realized by quantum annealing [32]. This relaxation voids the guarantee that the observed final state corresponds to the ground state of the problem Hamiltonian, although it may be sufficiently close in practice. Devices that implement quantum annealing to return minimum energy solutions can be referred to as quantum annealers.

QUANTUM COMPUTING ACROSS SCALES

Over the last few years, there has been an increased momentum to develop QC devices by many technology companies and start-ups using different models of quantum computation [33]. Several QC devices have also been made commercially available. However, these quantum computers are not fully practically viable due to their small scale. There has been a large influx of capital into the development of large-scale quantum computers to overcome the limitations faced by current quantum devices. A quantum system is required to be perfectly isolated from the outside world in order to use it for storing and processing information. However, the fragile nature of qubits and the absence of ideal surrounding conditions may result in the loss of information from the quantum system into the environment. This phenomenon is referred to as qubit decoherence [34]. Computations in quantum devices are performed by manipulating the quantum states within the QPU through external influence achieved by sophisticated control systems. This means that the model of quantum computation governing the QPU operation may also induce error or noise into the quantum system. A compromise in gate fidelity is a major hurdle in scaling up quantum circuit model devices and contributes additional quantum noise to the system. High-quality two-qubit gate operations are of utmost importance to achieve scalable quantum information processing [35]. Although quantum annealers impose less stringent requirements on qubit control than gate-based quantum computers, analog control errors may inhibit the scaling up of quantum annealers to a large number of qubits. In quantum annealers, errors associated with analog controls may widely vary the probability of obtaining the ground state of the problem Hamiltonian [36].

Protecting quantum systems against noise and scaling up QC devices is still a distant goal. The current quantum computers and the ones that may be available in the near future with more than 50 noisy qubits up to a few hundred can be collectively called noisy intermediate-scale quantum (NISQ) devices [18]. The current NISQ devices have an average two-qubit gate error rate of above 0.1%. Simply put, this means that more than 1,000 two-qubit gate operations cannot be performed in a quantum circuit without the noise overpowering the information present in the quantum system.

Many industries in the technology sector have been at the forefront of developing NISQ devices with the long-term goal of building scalable quantum systems that are less prone to quantum noise. As of the year 2021, quantum computers designed by IBM with 65 qubits, Honeywell with ten qubits, and Google with 54 qubits demonstrate similar gate errors, and all fall within the realm of NISQ, as shown in Fig. 3.

NISQ devices can be considered a stepping stone towards developing quantum computers with sufficiently low error rates capable of processing quantum information efficiently, termed fault-tolerant QC. Scalable fault-tolerant devices can be realized using quantum error correction principles [37]. Quantum error correction is essential, especially for efficient implementation of quantum algorithms at large scales to help mitigate errors associated with noisy qubits, faulty gates, and imprecise measurements. Error correction for quantum annealers has also been demonstrated to improve their performance substantially [38]. The number of qubits, along with their error rates, influences the capabilities of a quantum computer and can be quantified with the quantum volume metric [39]. As shown in Fig. 3, the quantum volume of fault-tolerant quantum computers increases with the better error-corrected qubits. Quantum error correction schemes pave the way towards achieving scaling speedups using large-scale noise-resilient quantum hardware for useful applications of practical relevance.

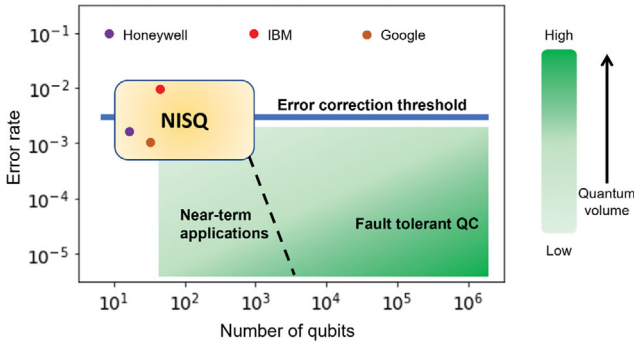

Fig. 3. Quantum computing across scales ranging from NISQ devices to fault-tolerant QC.

IMPACT OF QC IN THE NEAR-TERM

Although NISQ devices impose certain limitations on the computational power and fail to meet the requirements for fault-tolerant QC [40], they open up new frontiers for engineering applications through the testing of QC devices under experimental conditions. NISQ devices offer a unique platform to characterize quantum physical systems through control of quantum mechanical phenomena of qubit superposition and entanglement. This is a rather significant milestone since the existing powerful digital supercomputers cannot simulate quantum systems beyond the qubit threshold in NISQ devices [41]. Additionally, NISQ devices also allow for validation and evaluation of the performance of quantum algorithms that may constitute various QC applications. Noisy QC devices have already been shown to outperform classical computers for certain tasks, like the demonstration of Google's NISQ computer to achieve quantum supremacy [3]. Such advancements with NISQ devices illustrate the potential of quantum technologies for improving the state-of-the-art of several chemical engineering applications.

1. Optimization in the NISQ Era

Optimization problems in chemical engineering span across various scales and complexities, ranging from linear to nonlinear structures with both continuous and discrete variables. Optimization strategies to tackle such problems can be broadly categorized into mathematical programming techniques, random heuristics, and dynamic optimization [42]. Linear programming (LP) prob-

lems are linearly constrained optimization problems with continuous variables that can be generally solved in polynomial time [43]. However, many problems in the design and operations of chemical process systems involve discrete decisions, and they belong to the NP-hard complexity class [44,45]. Deterministic solution techniques based on mixed-integer programming (MIP) have been proposed to solve such complex problems [46], but often their computational complexity increases exponentially with problem size in the worst case. It should be noted that the complexity of an optimization strategy is measured in terms of the size of variables and input parameters of the problem, while the complexity of the problem is characterized by the best available solution algorithm's complexity. Quantum computers can solve optimization problems belonging to the bounded error quantum polynomial time (BQP) complexity class. BQP is the class of decision problems that can be solved by polynomial-time quantum computations with at most one-third probability of error [47]. Every classical circuit can be simulated by a quantum circuit [1], with AQC being computationally equivalent to the quantum circuit model [31]. LP problems in production planning [48], in principle, can be solved in polynomial time with either model of quantum computation. NP-hard problems are at least as difficult as NP-complete problems. The relationship between problem complexity classes is shown in Fig. 4. Despite the inflated publicity and hype revolving around the ability of QC to solve NP-hard problems, there is no evidence that quantum computers can even solve NP-complete problems efficiently [49]. These factors cast doubt on the ability of NISQ devices to outperform classical computers for even small-scale optimization problems. However, it should be noted that classical LP and MIP solvers like Gurobi and CPLEX are highly optimized for performance and make use of parallel computation in classical computers. Therefore, before applying quantum techniques for complex optimization problems in chemical engineering, it is crucial to determine whether or not such techniques can provide any advantage over classical algorithms or solvers either in terms of computational performance or quality of obtained solutions.

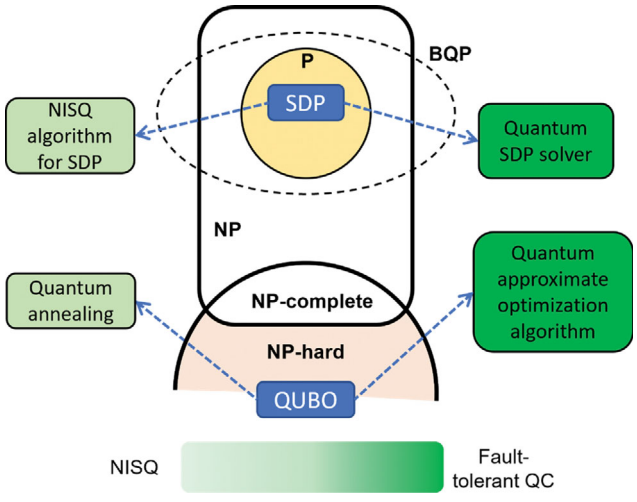

Fig. 4. Categorization of optimization problems like semidefinite programs (SDP) and quadratic unconstrained binary optimization problem (QUBO) problems solvable with quantum algorithms with both NISQ and fault-tolerant quantum devices along with the relationship between the polynomial time (P), nondeterministic polynomial time (NP), bounded error quantum polynomial time (BQP), NP-complete and NP-hard complexity classes.

Chemical engineering deals with chemical processes and unit operations that transform raw materials into useful products. As an alternative to experimentation, the design of complex materials like catalysts and other products that serve a certain functional purpose can be guided through advanced computational approaches like density functional theory [50], and other techniques in quantum chemistry applied using classical computers [51]. These approaches are designed to avoid maintaining an explicit wavefunction describing multi-particle characteristics because of the intractability stemming from its exponential growth on classical computers. Quantum computers can efficiently represent such wavefunctions as superposition of qubits' basis states [52]. Variational quantum eigensolver (VQE) is a quantum optimization algorithm that can be further applied to obtain the electronic configuration corresponding to the ground state energy of a given molecule [53]. VQE is a type of variational quantum algorithm using a low-depth quantum circuit that depends on the parameters of the quantum gates or a parameterized quantum circuit (PQC) to estimate the appropriate cost function. The inputs to the VQE algorithm are a molecular Hamiltonian describing the wavefunction and a PQC with randomly initialized parameters. Within VQE, the objective is to minimize the expectation value of the Hamiltonian by iteratively updating the PQC's parameters. Each iteration of VQE includes the steps of computing the expectation value with the quantum circuit using the current set of parameters and using a classical optimizer to update the parameter values. The classical optimizer performs a gradient descent step by computing gradients of the expectation value with respect to the parameters. This iterative procedure is repeated until the ground state of the target Hamiltonian or the minimum expectation value of the Hamiltonian is obtained. Key advantages offered by VQE include better compatibility with NISQ devices due to the absence of long coherent quantum circuits and resilience towards certain types of errors [54]. Such optimization approaches that allow for obtaining low-energy configurations in quantum chemistry applications demonstrate the high-computational power offered by NISQ devices despite the presence of quantum noise [55].

QC-based optimization techniques have also been proposed for certain classes of combinatorial optimization problems, namely, quadratic unconstrained binary optimization (QUBO) problems. QUBO problems appear in the fields of process systems scheduling [56], computer-aided design and planning [57], and many others [58]. QUBOs are NP-hard optimization problems, as shown in Fig. 4, that can generally be formulated by discretization and reformulation [59] or by mapping optimization problems as classic problems from theoretical computer science [60]. Quantum approximate optimization algorithm (QAOA) is another variational quantum algorithm that produces approximate solutions for the QUBO problems [61]. However, achieving a quantum speedup with QAOA over classical algorithms may require hundreds of qubits [62], rendering the QAOA algorithm implemented with NISQ devices

unsuitable for mid-size QUBO problems. In addition to algorithms for the quantum circuit model, quantum annealing implemented on an AQC platform inherently allows for finding low-energy solutions to the problem Hamiltonian describing the given QUBO problem. Before solving the optimization problem with a NISQ era quantum annealer, QUBOs are embedded onto the QPU according to the available architecture of qubits [63]. In comparison to meta-heuristics like simulated annealing, a larger probability of obtaining an optimal solution or ground state is exhibited by quantum annealing [32]. Apart from deterministic optimization methods, random heuristic approaches have also been applied to several chemical engineering applications [64]. Swapping quantum annealing-based approaches for other random search techniques in problems relevant to scheduling, manufacturing, and supply chain optimization could potentially be beneficial [22]. However, careful consideration regarding physical limits of NISQ devices is crucial to achieve speedups over classical optimization strategies.

2. Machine Learning in the NISQ Era

Machine learning refers to statistical models that can learn from experience by discovering patterns in data without rule-based programming. Many years of simulations and experiments in chemical engineering have led to a massive amount of data that can be used to train machine learning models, thus allowing for added flexibility, accuracy, and execution speed over traditional models and methods. Advances in areas of machine learning like deep learning and reinforcement learning have already revolutionized significant applications in bioinformatics, molecular modeling, process control, and many more [65]. Although the future of machine learning in chemical engineering applications holds promise, many classical machine learning techniques do not scale well with the amount of data and its dimensions. Optimization lies at the heart of machine learning that deals with minimizing the generalization error defined as a measure of erroneous predictions on previously unseen data. With the realization of quantum devices and the proposal of quantum algorithms to achieve speedups over their classical counterparts, research interest in quantum machine learning (QML) has grown to adopt quantum technologies to overcome issues faced by classical machine learning models. Several QML techniques have already been proposed in the literature with claims of quantum advantages [66] and are shown in Fig. 5. In addition to categorizing QML techniques into supervised, unsupervised, reinforcement learning tasks in Fig. 5, we also arrange them according to their compatibility with NISQ and fault-tolerant devices. The radius of the arc indicates the extent of the need for error correction to adopt the QML techniques within the arc for practical purposes. However, weighing the theoretical speedups against non-idealities of quantum systems is necessary before their practical implementation in chemical engineering applications at varying scales.

Training of machine learning models requires the use of high-quality data for their efficient operation. Quantum computers hold the possibility of accelerating the processing of high volumes of data as well as the training process by inducing a quantum speedup over classical algorithms. Quantum learning machines can represent and generalize data with both classical and quantum mechanical origins [67]. This can be achieved by encoding data in qubit

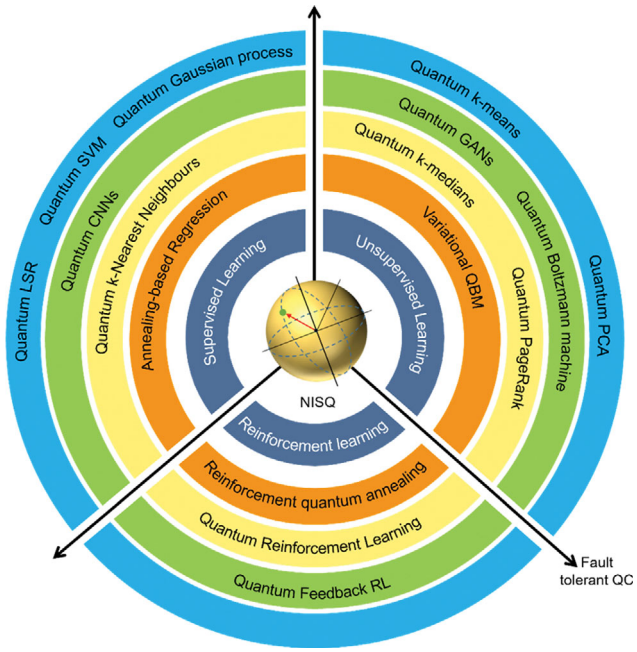

Fig. 5. Quantum machine learning techniques are categorized into machine learning tasks and arranged according to compatibility with NISQ and fault-tolerant devices.

states that results in a compact representation using a limited number of qubits and quantum gates with NISQ devices. An example of such data encoding can be seen for embedding a molecule's wavefunction as a quantum state to locate its low energy configurations in Section 4.1. Several QML techniques used for classification, like variational quantum classifier [68] and quantum-enhanced SVM [69], use quantum feature embedding or data encoding as an important subroutine. In general, data-driven QML techniques may use quantum feature embedding to encode available data for the rich, expressive power of developed quantum circuits [70]. Big data collected from many sectors of the chemical engineering community is high-dimensional [71], and processing it with such quantum data encoding schemes may prove beneficial even on NISQ devices by reducing the number of required operations. However, although the advantage of some QML methods stems from quantum data encoding, they may include other quantum computations that may not be suitable to perform on NISQ devices.

The three branches of machine learning are supervised, unsupervised, and reinforcement learning, as shown in Fig. 5. Supervised learning deals with generalizing from labeled data and involves tasks like classification for discrete value predictions and regression for continuous value predictions. As mentioned, variational quantum classifier [68] and quantum-enhanced SVM [69] are QML models for binary classification. In addition to using quantum feature embedding, these models use low-depth PQCs, thus enabling their use on NISQ devices. The variational quantum classifier is also referred to as quantum neural network (QNN) by drawing on the similarities between neural networks as a parameterized network and PQC. The underlying idea behind QNN is the use of PQC as a function approximator that estimates the cost or objective function of a specific machine learning task for the given

input data. Gradients of the estimated cost with respect to PQC's parameters can be easily obtained due to the application of unitary transformations defined by the quantum gates in the PQC. Classical optimizers like stochastic gradient descent can then be used to update the parameters of PQC with appropriate learning rates. Similar to the training of neural networks, this iterative procedure is repeated until the cost function converges to a local minimum. Variants of QNN like quantum convolutional neural networks (QCNN) utilize efficient parameterization with fewer parameters than their classical counterpart and allow for efficient training and implementation on realistic, near-term quantum devices [72]. These quantum classifiers could be used for applications ranging from object detection to fault diagnosis in chemical industrial processes [73]. Least-squares regression models and their variants are still highly relevant in chemical engineering and are a first step in describing the relationship between response variables like quality of a product or duration of a production process and may benefit extensively by the quantum speedup offered by quantum linear regression. Performing linear regression involves solving a system of linear equations. The Harrow-Hassidim-Lloyd (HHL) quantum algorithm provides an exponential speedup over classical algorithms for solving a system of linear equations [74]. Quantum algorithms for variants of least-squares regression (LSR) like quantum LSR also utilize HHL as an important subroutine [75,76]. However, any quantum advantage offered by HHL is application-specific and may be lost during the retrieval of solutions [77]. Since HHL is not suited for NISQ devices, the system of linear equations could be solved with the variational quantum linear solver (VQLS) [78]. Similar to VQE, VQLS is a variational quantum algorithm that employs low-depth quantum circuits at the expense of additional classical optimization. This trade-off is useful when using NISQ devices without error correction. Apart from the circuit model, regression tasks can also be performed with quantum annealers facilitated by an AQC platform [79]. Annealing-based regression has been applied to computational biology [80] and may have similar implications for molecular modeling and materials design in chemical engineering.

Apart from supervised machine learning methods, QML models have also seen advancements in unsupervised learning that learn patterns from untagged data when class labels are unavailable. Quantum generative adversarial network (QuGAN) is a quantum variant of a popular deep learning architecture for unsupervised learning tasks of generative modeling and uses PQCs like any quantum neural network architecture [81]. Quantum Boltzmann machines (QBMs) can learn complex data distributions [82] better than Boltzmann machines that serve as the basis of powerful deep learning models. Variational QBM is its variant developed to run on NISQ devices [83]. QBM inspired architectures trained with quantum annealing processors have been used for fault diagnosis in complex industrial processes and could be potentially applied in chemical industries [73,84]. PQCs have also been used as function approximators for value functions in reinforcement learning tasks for sequential decision making [85]. Such reinforcement learning algorithms can be deployable on near-term NISQ devices and scalable for large-scale process control applications in chemical engineering.

LONG-TERM IMPACT OF QC

Efficient error correction that allows for recovering from quantum errors even with the presence of noise within the quantum device's individual components should lead to the fault-tolerant QC era. The development of scalable fault-tolerant quantum computers will have major implications in fields such as engineering, experimental physics, computational chemistry, and many more. It has been speculated that fault-tolerant QC devices may be able to easily simulate any quantum mechanical phenomenon in nature at intermediate length scales [86]. Quantum algorithms that may be useful for practical applications in the future and have been proven to outperform classical algorithms substantially may require a very large number of qubits and gates. For example, factoring an integer represented by ten bits requires at least 42 qubits with high fidelity gates and measurement operators. Fault-tolerant computers capable of mitigating errors accumulated from the noisy qubits and quantum gates should be able to perform such large-scale quantum computations for chemical engineering applications with error-correcting quantum codes [87].

1. Optimization in the Fault-tolerant Era

Quantum chemistry simulation for materials design is one of the most promising applications of quantum computers, as the noise present in quantum systems is representative of the physical environment in which the simulated molecule exist. VQE algorithm is capable of exploiting the errors as features by using low-depth circuits to determine the electronic configuration of a molecule in its ground state. As of now, the largest computational chemistry problem involving 12 hydrogen atoms and a diazene molecule was solved and validated on a current quantum computer by making use of 12 and 10 qubits, respectively, and up to 72 two-qubit gates [88]. Similarly, to perform quantum chemistry simulations for general-purpose molecules like penicillin would potentially use approximately 286 qubits and 160 qubits for caffeine with high-depth circuits. Applications involving the design of drugs to target a specific disease pathway, new materials for electronics, and large molecules like polymers would require scalable fault-tolerant quantum computers that are capable of lowering the overhead associated with long quantum computations.

Large-scale combinatorial optimization problems formulated as QUBO problems could also be efficiently solved with fault-tolerant quantum computers. QAOA is known for its performance improvement with the depth of the quantum circuit used [61]. Fault-tolerant devices, due to their ability to execute high depth circuits with minimal overhead on the hardware, may allow for the solution of NP-hard problems and assess any quantum advantage offered [89]. Such error-correcting approaches may even perform better for difficult instances of QUBO problems where quantum annealing fails due to small spectral gaps. In addition to binary optimization problems, semidefinite programs (SDP) that include both LPs and quadratically constrained convex optimization problems are often solved for the optimal control problems in process systems engineering. Since process control systems are expected to compute decisions frequently and quickly especially for stable and sustainable operation of chemical plants, it is crucial to develop optimization strategies that can efficiently tackle SDP problems at

larger scales. Quantum improvements to SDP solution techniques like [90] and [91] require extensive quantum resources to provide a speedup. Fault-tolerant computers may help achieve the desired quantum speedups while solving large-scale SDPs, as shown in Fig. 4, that are otherwise intractable to solve on classical computers due to their exponential scaling.

2. Machine Learning in the Fault-tolerant Era

Distance-based machine learning techniques like nearest neighbor and k-means have been extensively applied to fault monitoring and outlier detection in process monitoring. In quantum variants of these methods, we point out that despite using quantum feature embedding as a subroutine, such QML techniques may fail to gain an advantage on NISQ devices mainly due to the use of Grover's search [92] to locate minima among computed distances. Training sets of modest size may require more than 15 qubits with error correction to perform Grover's search with high fidelity. One such QML technique for classification is the quantum k-nearest neighbor [69]. The quantum algorithm for k-means clustering can be implemented by encoding quantum data to quantum states, followed by Grover's search routine that locates the quantum state with minimum Euclidean distance [93]. Possible applications of clustering can be observed in process monitoring and control. Efficient training and inference of such QML methods for these applications would require error-corrected qubits in fault-tolerant devices, as summarized in Fig. 5.

The qubit requirement for HHL algorithm is to solve a system of linear equations in least-squares regression scales logarithmically with the number of data points in the training set. In addition, HHL uses quantum phase estimation as a subroutine that is severely constrained by low reliability and high variability of near-term quantum devices. An exponential speedup with HHL can be obtained for linear regression tasks [75,76] implemented on fault-tolerant devices even with exponentially large datasets [94]. For another variant of quantum SVM, referred to as qSVM, a least-square SVM formulation is solved by converting the inequality constraints in the primal SVM formulation into equalities by introducing slack variables [95]. This reduces the least-squares SVM problem to a system of linear equations that can also be efficiently solved with the HHL algorithm on fault-tolerant devices. Quantum Gaussian process regression is a Bayesian variant of linear regression that also requires matrix inversion in HHL [96]. The core component of a widely used dimensionality reduction technique, called principal component analysis (PCA), is the eigenvalue decomposition of the covariance matrix. In quantum PCA, spectral decomposition of the covariance matrix is performed by use of quantum phase estimation algorithm followed by the extraction of principal components by making measurements on the final state [97]. Chemical engineering applications have long-established the use of such dimensionality reduction techniques to overcome the curse of dimensionality and demonstrate exponential speedup in areas like process monitoring, chemometrics, and optimal control for energy management. A quantum reinforcement learning (QRL) framework that actually exploits quantum properties of superposition and entanglement and not just PQC as function approximators has been proposed well before the physical realization of any quantum computer [98]. This approach also makes use of Grover's iteration to determine optimal decisions but would require fault-tolerant quantum devices for its implementation. QRL-based approaches could enhance the performance of process control as well as other chemical engineering applications like materials design.

CONCLUSION

This article presents the challenges and opportunities of applying QC technologies for chemical engineering applications over various sectors. We provide a brief primer on different quantum computer operations and their shortcomings brought on by lack of technological maturity. Measures taken to mitigate noise present in quantum systems are also presented. The physical realization of near-term quantum computers with lower fidelity should not be dismissed since NISQ devices are a significant milestone on the road towards fault-tolerant QC. We provide insights into the use of quantum algorithms for specific areas in chemical engineering with both NISQ and fault-tolerant QC devices. Optimization and machine learning are used as the basis to classify and review corresponding quantum techniques. This article intends to inform the readers of the potential of QC, its challenges, and its advantages in a practical setting within the context of chemical engineering and consequently spark innovative, intuition-based, and scalable quantum solutions for complex problems in chemical engineering-related fields.

REFERENCES

1. M. A. Nielsen and I. Chuang, *Quantum computation and quantum information*, American Association of Physics Teachers (2002).
2. N. Friis, O. Marty, C. Maier, C. Hempel, M. Holzäpfel, P. Jurcevic, M. B. Plenio, M. Huber, C. Roos, R. Blatt and B. Lanyon, *Phys. Rev. X*, **8**, 021012 (2018).
3. F. Arute, K. Arya, R. Babbush, D. Bacon, J. C. Bardin, R. Barends, R. Biswas, S. Boixo, F. G. Brandao and D. A. Buell, *Nature*, **574**, 505 (2019).
4. A. Montanaro, *npj Quantum Inf.*, **2**, 15023 (2016).
5. S. Imre and F. Balazs, *Quantum computing and communications: an engineering approach*, John Wiley & Sons (2005).
6. R. Orús, S. Mugel and E. Lizaso, *Rev. Phys.*, **4**, 100028 (2019).
7. M. Ying, *Artif. Intell.*, **174**, 162 (2010).
8. R. P. Feynman, *Simulating physics with computers*, CRC Press (2018).
9. P. Benioff, *J. Stat. Phys.*, **22**, 563 (1980).
10. S. Gamble, in *Frontiers of engineering: Reports on leading-edge engineering from the 2018 symposium*, National Academies Press (2019).
11. R. Raz and A. Tal, in Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing (2019).
12. M. Fingerhuth, T. Babej and P. Wittek, *PloS One*, **13**, 0208561 (2018).
13. G. Garnier, *Front. Chem.*, **2**, 17 (2014).
14. L. T. Biegler, I. E. Grossmann and A. W. Westerberg, *Systematic methods for chemical process design*, Prentice Hall, Old Tappan, NJ (1997).
15. S. Dutta, *Optimization in chemical engineering*, Cambridge University Press (2016).
16. V. Venkatasubramanian, *AIChE J.*, **65**, 466 (2019).

17. C. Shang and F. You, *Engineering*, **5**, 1010 (2019).
18. J. Preskill, *Quantum*, **2**, 79 (2018).
19. S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin and X. Yuan, *Rev. Mod. Phys.*, **92**, 015003 (2020).
20. T. T. Tran, M. Do, E. G. Rieffel, J. Frank, Z. Wang, B. O'Gorman, D. Venturelli and J. C. Beck, in Ninth annual symposium on combinatorial search (2016).
21. S. Harwood, C. Gambella, D. Trenev, A. Simonetto, D. Bernal and D. Greenberg, *IEEE Trans. Quantum Eng.*, **2**, 1 (2021).
22. A. Ajagekar, T. Humble and F. You, *Comput. Chem. Eng.*, **132**, 106630 (2020).
23. B. Omer, Master's thesis, Institute of Information Systems Technical University of Vienn na (2000).
24. K. A. Britt and T. S. Humble, *ACM J. Emerging Technol. Comput. Syst.*, **13**, 1 (2017).
25. D. E. Deutsch, *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, **425**, 73 (1989).
26. A. Adedoyin, J. Ambrosiano, P. Anisimov, A. Bärtschi, W. Casper, G. Chennupati, C. Coffrin, H. Djidjev, D. Gunter and S. Karra, arXiv preprint arXiv:1804.03719 (2018).
27. C. C. McGeoch, *Synthesis Lectures on Quantum Computing*, **5**, 1 (2014).
28. D. J. Griffiths and D. F. Schroeter, *Introduction to quantum mechanics*, Cambridge University Press (2018).
29. T. Albash and D. A. Lidar, *Rev. Mod. Phys.*, **90**, 015002 (2018).
30. E. Farhi, J. Goldstone, S. Gutmann and M. Sipser, arXiv preprint quant-ph/0001106 (2000).
31. D. Aharonov, W. Van Dam, J. Kempe, Z. Landau, S. Lloyd and O. Regev, *SIAM Rev.*, **50**, 755 (2008).
32. T. Kadowaki and H. Nishimori, *Phys. Rev. E*, **58**, 5355 (1998).
33. "Final Report: Emerging Technologies Subcommittee Quantum Information Science", Homeland Security Advisory Council.
34. D. M. Bacon, *Decoherence, control, and symmetry in quantum computers*, University of California, Berkeley (2001).
35. Y. Xu, J. Chu, J. Yuan, J. Qiu, Y. Zhou, L. Zhang, X. Tan, Y. Yu, S. Liu and J. Li, *Phys. Rev. Lett.*, **125**, 240503 (2020).
36. A. Pearson, A. Mishra, I. Hen and D. A. Lidar, *npj Quantum Inf.*, **5**, 1 (2019).
37. D. Gottesman, arXiv preprint arXiv:0904.2557 (2009).
38. K. L. Pudenz, T. Albash and D. A. Lidar, *Nat. Commun.*, **5**, 3243 (2014).
39. A. W. Cross, L. S. Bishop, S. Sheldon, P. D. Nation and J. M. Gambetta, *Phys. Rev. A*, **100**, 032328 (2019).
40. D. Gottesman, *Phys. Rev. A*, **57**, 127 (1998).
41. S. Boixo, S. V. Isakov, V. N. Smelyanskiy, R. Babbush, N. Ding, Z. Jiang, M. J. Bremner, J. M. Martinis and H. Neven, *Nat. Phys.*, **14**, 595 (2018).
42. L. T. Biegler and I. E. Grossmann, *Comput. Chem. Eng.*, **28**, 1169 (2004).
43. J. A. Kelner and D. A. Spielman, in Proceedings of the thirty-eighth annual ACM symposium on Theory of computing (2006).
44. I. E. Grossmann and A. W. Westerberg, *AIChE J.*, **46**, 1700 (2000).
45. K. C. Furman and N. V. Sahinidis, *Comput. Chem. Eng.*, **25**, 1371 (2001).
46. I. E. Grossmann and L. T. Biegler, *Comput. Chem. Eng.*, **28**, 1193 (2004).
47. E. Bernstein and U. Vazirani, *SIAM J. Comput.*, **26**, 1411 (1997).
48. S. S. Rao, *Engineering optimization: Theory and practice*, John Wiley & Sons (2019).
49. S. Aaronson, *SIGACT News*, **36**, 30 (2005).
50. R. G. Parr, *Density functional theory of atoms and molecules*, in Horizons of quantum chemistry, Springer (1980).
51. T. Helgaker, W. Klopper and D. P. Tew, *Mol. Phys.*, **106**, 2107 (2008).
52. Y. Cao, J. Romero, J. P. Olson, M. Degroote, P. D. Johnson, M. Kieferová, I. D. Kivlichan, T. Menke, B. Peropadre and N. P. Sawaya, *Chem. Rev.*, **119**, 10856 (2019).
53. A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik and J. L. O'brien, *Nat. Commun.*, **5**, 1 (2014).
54. B. Bauer, S. Bravyi, M. Motta and G. K.-L. Chan, *Chem. Rev.*, **120**, 12685 (2020).
55. M. P. Andersson, M. N. Jones, K. V. Mikkelsen, F. You and S. S. Mansouri, *Curr. Opin. Chem. Eng.*, **36**, 100754 (2022).
56. B. Alidaee, G. A. Kochenberger and A. Ahmadian, *Int. J. Syst. Sci.*, **25**, 401 (1994).
57. J. Krarup and P. M. Pruzan, *Computer-aided layout design*, in Mathematical programming in use, Springer (1978).
58. G. Kochenberger, J.-K. Hao, F. Glover, M. Lewis, Z. Lü, H. Wang and Y. Wang, *J. Comb. Optim.*, **28**, 58 (2014).
59. A. Ajagekar and F. You, *Energy*, **179**, 76 (2019).
60. A. Lucas, *Front. Phys.*, **2**, 5 (2014).
61. E. Farhi, J. Goldstone and S. Gutmann, arXiv preprint arXiv:1411.4028 (2014).
62. G. G. Guerreschi and A. Y. Matsuura, *Sci. Rep.*, **9**, 1 (2019).
63. R. Patton, C. Schuman and T. Potok, *Quantum Inf. Process.*, **18**, (2019).
64. J. Li and R. R. Rhinehart, *Comput. Chem. Eng.*, **22**, 427 (1998).
65. J. H. Lee, J. Shin and M. J. Realff, *Comput. Chem. Eng.*, **114**, 111 (2018).
66. J. Biamonte, P. Wittek, N. Pancotti, P. Rebentrost, N. Wiebe and S. Lloyd, *Nature*, **549**, 195 (2017).
67. E. Aïmeur, G. Brassard and S. Gambs, *Machine learning in a quantum world. In conference of the canadian society for computational studies of intelligence*, Springer, Berlin, Heidelberg (2006).
68. E. Farhi and H. Neven, arXiv preprint arXiv:1802.06002 (2018).
69. N. Wiebe, A. Kapoor and K. Svore, arXiv preprint arXiv:1401.2142 (2014).
70. M. Schuld, R. Sweke and J. J. Meyer, *Phys. Rev. A*, **103**, 032430 (2021).
71. L. Chiang, B. Lu and I. Castillo, *Annu. Rev. Chem. Biomol. Eng.*, **8**, 63 (2017).
72. I. Cong, S. Choi and M. D. Lukin, *Nat. Phys.*, **15**, 1273 (2019).
73. A. Ajagekar and F. You, *Comput. Chem. Eng.*, **143**, 107119 (2020).
74. A. W. Harrow, A. Hassidim and S. Lloyd, *Phys. Rev. Lett.*, **103**, 150502 (2009).
75. M. Schuld, I. Sinayskiy and F. Petruccione, *Phys. Rev. A*, **94**, 022342 (2016).
76. Y. Liu and S. Zhang, *Theor. Comput. Sci.*, **657**, 38 (2017).
77. S. Aaronson, *Nat. Phys.*, **11**, 291 (2015).
78. C. Bravo-Prieto, R. LaRose, M. Cerezo, Y. Subasi, L. Cincio and P. Coles, *Bull. Am. Phys. Soc.*, 65 (2020).
79. C. C. Chang, A. Gambhir, T. S. Humble and S. Sota, *Sci. Rep.*, **9**, 1 (2019).

80. R. Y. Li, R. Di Felice, R. Rohs and D. A. Lidar, *npj Quantum Inf.*, **4**, 14 (2018).
81. S. Lloyd and C. Weedbrook, *Phys. Rev. Lett.*, **121**, 040502 (2018).
82. M. H. Amin, E. Andriyash, J. Rolfe, B. Kulchytskyy and R. Melko, *Phys. Rev. X*, **8**, 015002 (2018).
83. C. Zoufal, A. Lucchi and S. Woerner, *Quantum Mach. Intell.*, **3**, 7 (2021).
84. A. Ajagekar and F. You, *Appl. Energy*, **303**, 117628 (2021).
85. S. Y.-C. Chen, C.-H. H. Yang, J. Qi, P.-Y. Chen, X. Ma and H.-S. Goan, *IEEE Access*, **8**, 141007 (2020).
86. J. Preskill, *Fault-tolerant quantum computation, in Introduction to quantum computation and information*, World Scientific (1998).
87. E. T. Campbell, B. M. Terhal and C. Vuillot, *Nature*, **549**, 172 (2017).
88. F. Arute, K. Arya, R. Babbush, D. Bacon, J. C. Bardin, R. Barends, S. Boixo, M. Broughton, B. B. Buckley and D. A. Buell, *Science*, **369**, 1084 (2020).
89. L. Zhou, S.-T. Wang, S. Choi, H. Pichler and M. D. Lukin, *Phys. Rev. X*, **10**, 021067 (2020).
90. F. G. Brandao and K. M. Svore, in Annual Symposium on Foundations of Computer Science (FOCS), IEEE (2017).
91. J. van Apeldoorn and A. Gilyén, arXiv preprint arXiv:1804.05058 (2018).
92. L. K. Grover, in *Proceedings of the twenty-eighth annual ACM symposium on Theory of Computing*, Association for Computing Machinery, Philadelphia, Pennsylvania, USA (1996).
93. S. Lloyd, M. Mohseni and P. Rebentrost, arXiv preprint arXiv: 1307.0411 (2013).
94. N. Wiebe, D. Braun and S. Lloyd, *Phys. Rev. Lett.*, **109**, 050505 (2012).
95. P. Rebentrost, M. Mohseni and S. Lloyd, *Phys. Rev. Lett.*, **113**, 130503 (2014).
96. Z. Zhao, J. K. Fitzsimons and J. F. Fitzsimons, *Phys. Rev. A*, **99**, 052331 (2019).
97. S. Lloyd, M. Mohseni and P. Rebentrost, *Nat. Phys.*, **10**, 631 (2014).
98. D. Dong, C. Chen, H. Li and T. Tarn, *IEEE Trans. Syst. Man Cybern. Part B Cybern.*, **38**, 1207 (2008).

Professor Fengqi You is currently Roxanne E. and Michael J. Zak Professor in Cornell University, Ithaca, New Yok, USA. He also serves as Chair of PhD Studies in Cornell Systems Engineering, Associate Director of Cornell Energy Systems Institute, and Associate Director of Cornell Institute for Digital Agriculture. He has published more than 200 refereed articles in journals such as *Science*, *Nature Sustainability*, *Nature Communications*, and *Science Advances*, and has an *h*-index of 65. He is an award-winning scholar and teacher, and has received over 15 major awards over the past five years from from the American Institute of Chemical Engineers (AIChE), American Chemical Society (ACS), Royal Society of Chemistry (RSC), American Society for Engineering Education (ASEE), and American Automatic Control Council (AACC) to recognize his research and educational accomplishments, in addition to a number of best paper awards. He is currently an editor of *Computers & Chemical Engineering*, an associate editor of AAAS journal *Science Advances* and of *IEEE Transactions on Control Systems Technology*, a consulting editor of *AIChE Journal*, and an editorial board member of *ACS Sustainable Chemistry & Engineering*, *Industrial & Engineering Chemistry Research*, *IEEE Quantum Computing Newsletter, PRX Energy, etc.*