FOSSIL ENERGY WORKSHOP ON QUANTUM INFORMATION SCIENCE & TECHNOLOGY SUMMARY REPORT

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WORKSHOP CHARGE/SCOPE

Quantum Information Science (QIS) is expected to profoundly change the practice of science and engineering in the coming decades. It is a rapidly progressing field, fueled by large investments from the private sector and governments. Its importance to the U.S. economy and national security is underscored by the National Quantum Initiative Act passed in December 2018[1]. QIS includes quantum sensing, quantum communications, quantum simulation experiments, and quantum computation. QIS technology exploits quantum phenomena for performing tasks that are impossible to do today, such as finding prime factors of large numbers or elucidating reaction mechanisms in complex chemical systems.

The opportunities for applying QIS to problems encountered in fossil energy technology development are not known today. This workshop brought together, for the first time, experts in these fields to exchange information and explore potential research opportunities for QIS to advance fossil energy. The goal of the workshop was to develop a set of priority research opportunities that can inform future research efforts in QIS and build a community of next-generation researchers at the intersection of QIS and fossil energy.

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EXECUTIVE SUMMARY

This workshop was one of the recommendations in a strategic plan that the National Energy Technology Laboratory (NETL) and DOE Office of Fossil Energy (FE) jointly developed to determine the near- and mid-term opportunities for the application of quantum information science (QIS) to fossil energy. The workshop goal was to develop a set of priority research opportunities that can inform future research efforts in QIS and build a community of next-generation researchers at the intersection of QIS and fossil energy. It brought together fossil energy and QIS experts from industry, academia, and national laboratories. The workshop participants discussed QIS applications in four panel discussions: Quantum Sensors/Detectors and Quantum Experiments; Quantum Computation for Machine Learning, AI, and Optimization; Quantum Computation/Simulation for Chemistry and Materials; and Quantum Computation for Process Modeling/CFD and Quantum Networking. The recommendations emanating from the workshop are reported here, organized by the relevant fossil energy technology development areas.

Quantum sensing has a shorter time to maturity and utility for fossil energy compared to other QIS areas such as fault-tolerant quantum computing. Quantum sensors exploit quantum mechanical properties to detect signals with higher signal-to-noise ratio than their classical sensor equivalents. Increasing the signal-to-noise ratio, a major goal of quantum sensing research, is accomplished through quantum light sources and detectors or atomic sensors that use populations of atoms rather than photons as the sensing field. Fiber optic sensors using *squeezed light*—with reduced uncertainty in its electric field strength in the phases used for the measurement at the expense of increased uncertainty in other phases—as the interrogating field could find applications in oil and gas extraction or carbon capture and storage. Measurements of interest include dynamic and static strain, magnetic fields, temperature, and others. Near-distance standoff photo-absorption techniques in the visible and near infrared spectral regions offer a potential method for detecting rare earth elements, another key fossil energy application.

Quantum entanglement—a quantum phenomenon (without a classical analog) that the state of each particle of a pair (or group) cannot be described independently of the state of the others, even when the particles (e.g., photons) are separated by large distances—can be exploited in quantum sensing. Entangling a minimum of two atomic clocks that are geographically separated is expected to increase the accuracy of the clocks. Sensors relying on time order, or sensors relying on ultrafast optics or dynamics can benefit from entangled atomic clocks. In general, sensors benefitting from a universal frame for time and frequency measurements will perform with more accuracy if entangled clocks can be distributed over geographically relevant sites for oil & gas exploration.

Another example is better assessment of Earth's gravitational field and thus local density of earth—according to *relativistic geodesy*, where gravity is measured at different locations on earth from measuring the rates of different clocks. Therefore, by invoking precision metrology afforded by the universal platform of time and frequency offered by entangled clocks, the frequency and amplitude of minute gravity oscillations associated with the breathing modes of earth may be detected. Ultrafast and ultraprecise detection of the extent of explosion and gravity fluctuations, stress variation (e.g., as a result of transient mechanical waves), presence of and displacement in fluids, etc., can be used for better design and control in mining.

In most cases, applicable quantum sensors could be brought to deployment within a few years. In the near term (0–3 years) we expect certain proof of principle laboratory-scale demonstrations to take place, in which squeezed light or entangled photons are used to enhance spectroscopy, standoff detection, and radar/lidar applications. Simultaneously, we expect advances to mitigate loss in fiber optic sensors that will make quantum fiber optic sensors viable in the medium (3–10 year) time frame. The most rigorous environments—well and subsurface applications—are expected to become feasible in the 10-year timeframe, though a combination of advances in quantum light sources, loss mitigation, and sensing protocols may move this timeline up considerably, by perhaps as much as 5 years.

Quantum sensing approaches for physical metrology and chemical sensing applied to field operations will offer opportunities to reduce the uncertainties in **subsurface** operations. This could have a large impact on energy production because the subsurface is the source of all fossil energy resources, which currently account for around 80% of the energy consumed worldwide. Quantum sensors could provide new insights into the interfacial molecular structure and macroscopic properties of common and novel fluids for subsurface operations, characterize the viscosity and chemical constituents of injectate and produced fluids at the surface and deep underground, and log borehole porosity.

The most important near-term goal in the application of QIS to **cybersecurity** should be to make fossil energy devices "quantum ready," not only for quantum key distribution (QKD) but also for general quantum communication and networking that provides benefits beyond cybersecurity. This goal includes integration with existing classical networks and standards such as, for example, General Electric's Digital Ghost, and perhaps, more specifically, to quantum-secure sensors. A quantum internet with interconnecting quantum sensors is a suggested goal for the short- and mid-term. The mid-term goals could be continued cost reduction and integrating quantum network security and sensing. In the longer-term, lessons learned from QKD in industry are critical for extending the quantum channel into a quantum internet, whose base technology is likely to be entanglement distribution. This effort should be pursued for quantum-secure interconnectivity among processors, sensors, and legacy systems.

Quantum simulation and **quantum computing** have applications in several different areas of fossil energy technology development. Quantum simulation involves using a "controllable quantum system to study another less controllable or accessible quantum system." Quantum simulation could be implemented with analog devices that would be easier to construct than quantum computers. Quantum computers use quantum bits, or qubits, which represent the values 0 or 1, or some combination of both at the same time (known as a *superposition*). Entangled qubits can access an exponentially larger parameter space compared with classical bits, enabling quantum computers to solve problems impossible on classical computers, such as finding prime factors of large numbers or elucidating reaction mechanisms in complex chemical systems.

Quantum computing and analog quantum simulators could accelerate the development of **materials** used in fossil energy technologies, such as catalysts for direct methane conversion, oxygen carriers for chemical looping processes, sorbents and solvents for carbon capture, and materials for the storage of chemical, thermal, and electrical energy. In the near-term, analog quantum simulators need to be explored for materials development. Quantum machine learning algorithms could accelerate the development of catalyst materials, which require a massive number of quantum computations. Inverse design of functional materials, which aims to develop materials with properties suitable for specific applications, could benefit from the speed of quantum computational algorithms.

A better understanding of both the potential benefits and challenges in the application of quantum computing to **powerplant design and optimization** is needed. Among the challenges is determining how to effectively map problems/data into quantum compatible forms and back to classical formulations to enable hybrid computing approaches. An exploratory research project among fossil energy optimization experts and quantum information scientists to develop effective mapping approaches for problems/data into quantum compatible forms and back to classical formulations would enable an interface between classical and quantum computing that could be used to rapidly demonstrate potential benefits of quantum computing on ongoing fossil energy systems optimization priorities.

Quantum computing could potentially address several needs in **power plant operation and control**, such as real-time optimization of fuel/air ratio, optimizing the operation of NOx and SOx control equipment, and improving the burner design. Quantum computing may also find applications in the compression of massive amounts of data generated by various process instruments and in using that high-fidelity data and enhanced understanding of real-time materials/chemistry and thermodynamics/heat transfer phenomena to make boiler component (e.g., tubes) life predictions. Another area that needs attention is the development of quantum performance benchmarks that are most relevant to fossil energy.

The development of workforce at the intersection of fossil energy and QIS could be initiated, for example, through NETL and Pittsburgh Quantum Institute collaborative interactions focused on QIS research in sensing, simulations, and networks applied to high priority fossil energy problems. Establishing flexible fellowship opportunities will help attract students to work at the intersection of fossil energy and QIS and gain expertise in QIS applications to fossil energy.

1. INTRODUCTION

1.1 Background

Quantum Information Science (QIS) is a rapidly progressing field with the potential to make revolutionary changes in many areas of science and engineering. This expectation and the exciting results from R&D to date have energized a large, worldwide effort in QIS R&D, funded by both industry and governments. In the U.S. a signature event has been the signing of the National Quantum Initiative Act into law in December 2018[1]. The Act launched ten years of sustained effort at the three lead agencies: National Institute of Standards and Technology (NIST), National Science Foundation (NSF) and DOE. It directs DOE to conduct a basic research program on QIS, leverage knowledge from existing QIS research, provide QIS training for additional undergraduate and graduate students, and coordinate research efforts with currently funded programs. It directs DOE Office of Science to establish two to five National Quantum Information Science Research Centers, which has resulted in a funding opportunity being announced in January 2020.

Quantum computing, a major area within QIS, has been embraced by some of the most influential technology companies in the world, such as Google, IBM, and Microsoft. It could enable computations that are presently impossible, such as finding prime factors of large numbers or elucidating reaction mechanisms in complex chemical systems. The era of quantum computing is said to have dawned in October 2019 when Google researchers reported that they had used a quantum computer to perform a calculation that cannot be done even on the fastest supercomputer in the world, reaching a milestone known as quantum supremacy[2, 3]. The rapid progress in quantum computing R&D is expected to accelerate the growth of the enterprise quantum computing market. It is expected that by 2023, 20% of organizations will be budgeting for quantum computing projects[4] and that by 2025, the worldwide annual budget for enterprise quantum computing will rise to $2.2 billion (from $39.2 million in 2017) led by pioneering industry users from the life sciences, aerospace, oil, gas, mining, agriculture, and automotive industries[5].

Given the rapid pace of development in QIS and its enormous promise, it became clear that National Energy Technology Laboratory (NETL) and DOE Office of Fossil Energy (DOE-FE) must assess the potential applications of QIS to fossil energy technology development. To that end, NETL initiated a strategic planning exercise in February 2019 and developed a strategic plan in April 2019. One of the recommendations in the strategic plan was to organize a workshop to determine the near- and mid-term opportunities for QIS applications in fossil energy, bringing together NETL/DOE-FE researchers and stakeholders and QIS experts from industry, academia, and national laboratories. Early on, Pittsburgh Quantum Institute joined the effort as a co-organizer of the workshop and shared their expertise in QIS to plan an effective workshop structure. The goal of the workshop was to develop a set of priority research opportunities that can inform future research efforts in QIS and build a community of next-generation researchers at the intersection of QIS and fossil energy.

1.2 Fossil Energy

1.2.1 Fossil Energy Will Remain the Foundation for World Energy Demand for Decades to Come

Fossil energy provides quality of life to millions of Americans, sustains America's manufacturing and high-technology industries, fuels economic growth, and stimulates technical innovation. Tremendous technological effort and innovation has diversified the energy portfolio to meet ever increasing global demand. Even so, studies project that fossil energy will be required to supply expanding world energy markets and will continue to satisfy nearly 80% of energy demand for decades[6].

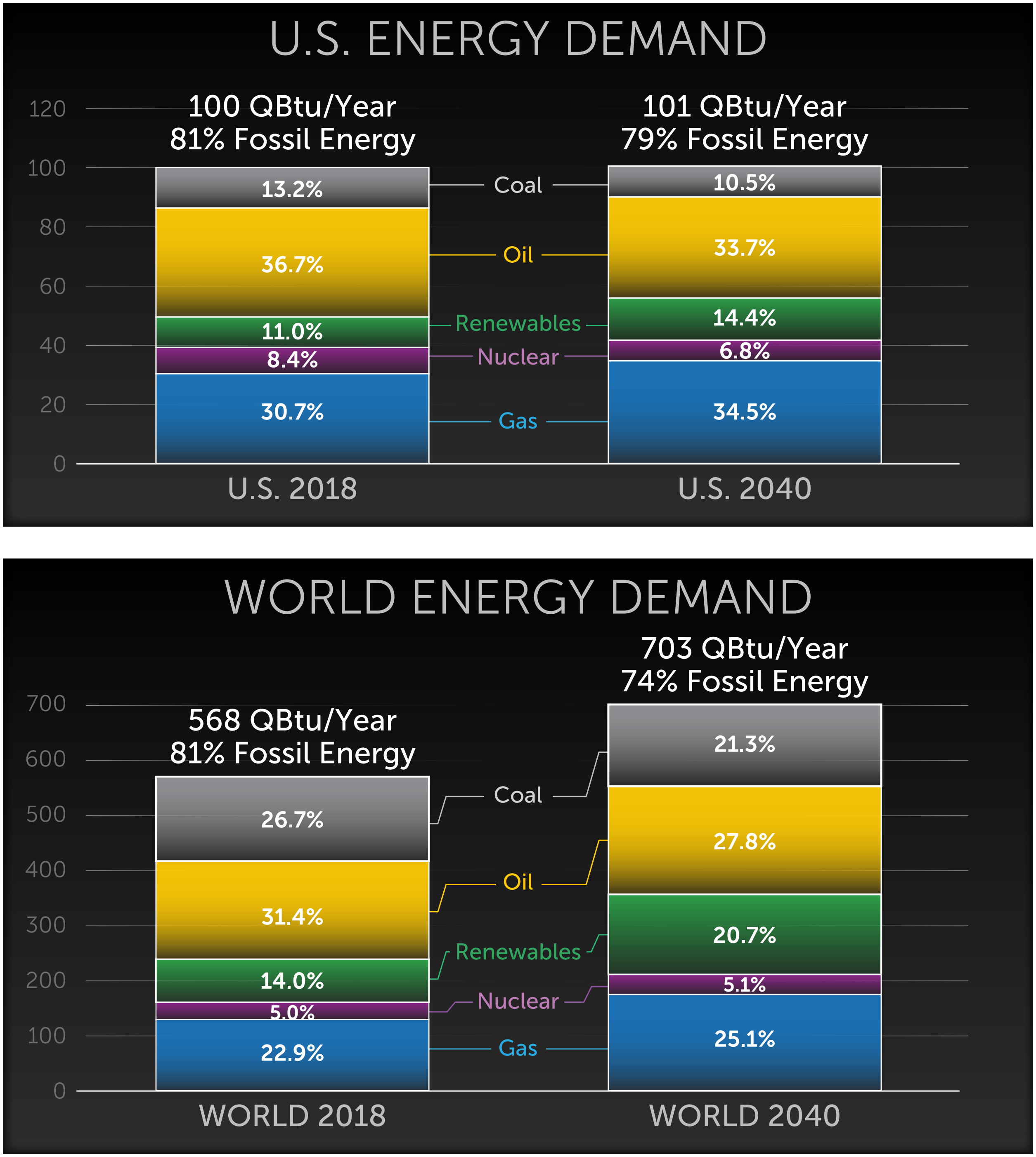


FIGURE 1. *World Energy Demand by Energy Source*[7,8].

Fossil fuel currently provides 60% and 58% of the U.S. and World's electricity, respectively. It is projected that by 2050 fossil fuel will continue to be the main source of fuel for electricity production both in the U.S. (50%) and worldwide (43%)[9].

1.2.2 Advanced Technologies Are Critical to the Future of Fossil Energy

Advanced technologies enable fossil fuels to produce the clean, reliable, and affordable energy needed to increase domestic manufacturing, invest in improving our Nation's energy infrastructure, improve electrical grid reliability and resilience, expand domestic energy production, and support U.S. energy and national security goals.

1.2.3 Fossil Energy Research Priorities

Six bold fossil energy research and development priorities have the potential to advance the Nation's entire energy system[10].

- Develop the coal plants of the future by advancing small-scale modular coal plants of the future, which are highly efficient and flexible with near-zero emissions
- Modernize the existing coal-fired fleet by improving its performance, reliability, and efficiency
- Reduce the cost and risk of carbon capture, utilization, and storage (CCUS) to enable wider deployment
- Advance big data by optimizing recovery of oil and gas resources with real-time analysis and machine learning
- Address the energy water nexus by improving efficient use of water resources
- Develop rare earth elements (REE) separation and recovery technologies and processes to manufacture valuable products from coal to address current global market and process economics

These research priorities are currently supported through initiatives such as [10]:

- Coal FIRST (Flexible, Innovative, Resilient, Small, Transformative), which is accelerating development of efficient, flexible, and cost-effective coal-fired power plants, while safely and cost-effectively enabling environmental stewardship of fossil energy-based conversion systems.
- The Science-Informed Machine Learning for Accelerated Real-Time (SMART) decisions in the subsurface initiative supports real-time analysis leading to dramatic improvements in subsurface visualization, dynamic forecasting, and autonomous control.
- Developing advanced sensors and controls to help increase coal plant efficiency, reduce forced outages, and avoid downtime related to equipment failures and compliance with environmental regulations.
- Exploring water-treatment technologies that reduce the amount of water needed for hydraulic fracturing and developing breakthrough shale-stimulation technologies that reduce water use.
- Developing new capture approaches and integration of capture with novel energy conversion such as chemical looping, oxycombustion, and direct cycle supercritical CO_2 systems to drive down the price of carbon capture.
- Developing technologies for recovery of REEs from coal and coal by-products such as process/production technologies, environmental management, sampling, characterization, and analysis, and system integration and optimization for producing REEs.
- Engineering extreme small-scale nano-materials or nano-sensors for injection into natural gas reservoirs to gather subsurface information far from the wellbore and using new modeling and simulation capabilities utilizing high-performance computing to interpret subsurface data.

1.3 Quantum Information Science (QIS)

The projected continued use of fossil energy value chain elements (extraction, transportation, conversation, and end-of-life use) makes it imperative that they be as efficient, economical, and clean as possible. QIS can play a critical role in achieving these goals as it enables integration of "quantum" concepts and techniques into existing and future research activities and technologies. QIS uses distinct behaviors of quantum systems and is expected to lay the foundation for the next generation of computing and information processing, as well as an array of other innovative technologies in sensing and related applications. QIS comprises four distinct areas:

1.3.1 Quantum Sensing[11]

Quantum sensing exploits the strong sensitivity of quantum systems to external disturbances to measure physical quantities such as magnetic or electric fields and/or to enhance the sensitivity of analytical measurements. Two prominent strategies may be exploited for quantum sensing: (1) The photonic quantum sensing exploits the quantum nature of light for enhancements in a range of applications, from remote target detection to the readout of optical memory. (2) Non-photonic quantum sensors, which rely on spin qubits, trapped ions, and other materials with well-defined quantum states that may be initialized, manipulated, and read-out using accessible analytical techniques, have also been developed for applications including magnetometry, thermometry, atomic clocks, and others. Quantum sensing is well developed for photonic applications among other advanced areas of quantum information mainly because quantum optics provide the most mature and convenient setting for implementing quantum metrology and quantum imaging without the need for cryogenic operational temperatures or other constrained operational conditions.

1.3.2 Quantum Networking

Quantum networking transmits information with the help of "entangled" particles whose quantum state cannot be described independently, even when they are separated by a large distance. The quantum enhanced communication protocols surpass the existing dominant protocols based upon the classical laws and offer a new paradigm in communications. A number of devices form a quantum network, which is capable of transmitting encrypted information using the laws of quantum mechanics, featuring entanglement-enabled quantum teleportation and paving the way for a quantum internet. For example, Argonne National Laboratory, Fermilab, and University of Chicago are partnering to "teleport" information across a 30-mile distance between the two labs. Quantum networking using quantum key distribution (QKD) methods enables secure transmission of data over distant networks preventing data exposure to unintended recipients.

1.3.3 Quantum Simulation[12]

Quantum simulation Involves using a "controllable quantum system" to study another less controllable or accessible quantum system. There are several proposals such as neutral atoms, ions, polar molecules, electrons in semiconductors, superconducting circuits, nuclear spins and photons that are proposed as possible quantum simulators. Experts currently believe that quantum simulations can be near- or mid- term opportunities, as quantum computers are in their early stage and lack maturity to perform computational work that cannot be done using classical computers. Potential applications include[13] materials science, catalyst development, molecular systems, and chemical reactions.

1.3.4 Quantum Computing[14]

Quantum computers use quantum mechanical phenomena such as superposition, interference, and entanglement to perform computations. Quantum computers use quantum bits, or qubits, which represent the values 0 or 1, or some combination of both at the same time (known as a "superposition"). A set of intrinsically interconnected ("entangled") qubits can access an exponentially larger parameter space than the same number of classical bits, enabling quantum computers to solve problems impossible to solve with classical computers. Potential applications include[15] Encryption and Cybersecurity, Financial Services, Drug Research and Development, Supply Chain Logistics, and Data Analysis and Machine Learning.

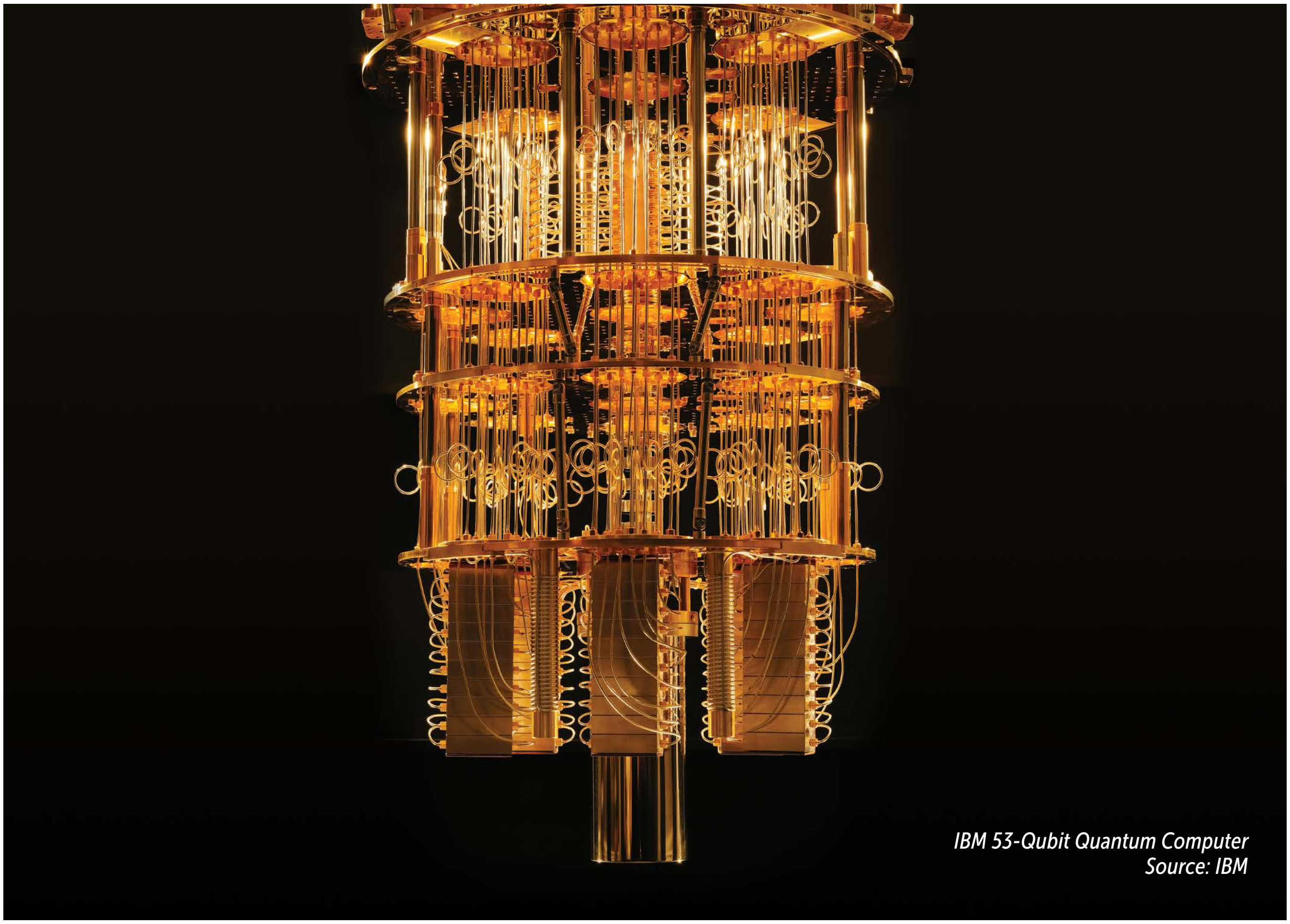
1.3.5 National Quantum Initiative Act

The importance of quantum information science to the U.S. economy and national security is underscored by the National Quantum Initiative Act, which was signed into law on 21 December 2018[1]. The legislation establishes a coordinated multiagency program in QIS and directs DOE, NSF, and NIST to support R&D and education in QIS, set program goals, and facilitate partnerships among federal laboratories, universities, companies, and other entities. The act establishes three mechanisms for coordinating and administering the initiative: the QIS subcommittee within the National Science and Technology Council, the National Quantum Initiative Advisory Committee, and a National Quantum Coordination Office to administer the initiative. They are mandated to continue their activities for 11 years and may be renewed thereafter at the prerogative of the president.

In accordance with the act the key agencies started receiving QIS R&D funding in the Fiscal Year 2020 (FY20). The Fiscal Year 2021 (FY21) budget request greatly bolsters the QIS R&D funding, increasing by over 50 percent compared to the FY20 budget on the path to double to over $860 million by 2022[16]. In FY21 the requested NSF funding for QIS would double to $230 million. The DOE Office of Science funding for QIS would increase from $195 million to $237 million[17]. DOE began soliciting proposals for the multidisciplinary QIS research centers in January 2020 and plans to select between two and five centers that will collectively receive up to $625 million over five years[17]. The DOE funding also includes $25 million to support early state research for a quantum internet. NIST funding would be $40 M, enabling it to focus on quantum networking and to support its nascent Quantum Economic Development Consortium and existing research institutes at the University of Colorado Boulder and the University of Maryland[18]. NASA's initial funding will allow it to explore the potential for a space-based quantum entanglement experiment[16]. The benefits are succinctly stated in the FY21 budget document: "QIS will improve our industrial base, creating new jobs and entirely new industries in the process, while helping keep America safe."[16]

2. ABOUT THE WORKSHOP

The workshop brought together 54 participants with expertise in a variety of relevant areas in fossil energy (33) and QIS (21). They came from DOE (2), industry (12), universities (17), and national labs (23). For the purposes of the workshop (and this report) fossil energy includes areas such as sensors, materials, optimization, modeling, artificial intelligence, machine learning, etc., that have applications in fossil energy technology development. The workshop began with three keynote talks, which were followed by four panel sessions and a facilitated brainstorming session [Appendix A]. The panel sessions focused on application-oriented topics aligned with areas of QIS. They produced a list of QIS application opportunities, priority research directions, workforce development ideas, and collaboration opportunities. The panel moderators reported on these topics at the beginning of the facilitated brainstorming session. From the ensuing discussions a list of topics to be considered in the workshop report was generated. These topics were reorganized by fossil energy application areas in consideration of the main audience of the workshop report: DOE-FE and NETL program management and researchers seeking opportunities for QIS applications to fossil energy technologies. The workshop report was written by a subset of the panel members who further refined and expanded upon the topics generated during the workshop.



IBM 53-Qubit Quantum Computer
Source: IBM

3. OBSERVATIONS: QIS APPLICATIONS TO FE TECHNOLOGIES

The following sections of this report focus on QIS concepts and techniques applicable to various FE technologies: Subsurface Systems; Sensors; Materials Development; Power Plant, Electrical Grid, and Oil & Gas Cybersecurity; Power Plant Design and Optimization; and Power Plant Operation and Control.

3.1 Sensors

A near-term application of quantum information science for fossil energy noted at the workshop was quantum sensing. Quantum sensors are devices that exploit quantum mechanical properties to detect signals with higher signal-to-noise ratio (SNR) or with shorter integration times for the same SNR as their classical sensor equivalents. These devices can make use of superposition, entanglement, or quantum noise reduction (squeezing). They may also rely on qubits as the probes or transduction mechanism. Quantum sensing has a shorter time to maturity and utility for fossil energy compared to fault-tolerant quantum computing, which is still some years away. However, quantum sensing addresses very different use cases than computing. Several areas of interest to the DOE-FE Office that overlap with applicable areas for quantum sensing were identified during the workshop. Not all candidate areas have quantum sensors readily available, but the possibility to modify classical sensors or to produce new quantum sensors for some of these areas exists. Focused research, development, engineering, and technology transfer of quantum sensors and sensing platforms will help overcome classically imposed sensing bottlenecks. These efforts will, in turn, yield a much richer sensing environment for a variety of applications of interest to DOE-FE including understanding of geological processes, exploration of unconventional oil and gas fields, discovery of untapped rare earth mineral deposits, and improvements in mine safety.

Many sensors are approaching their ultimate classical noise limits due to the Heisenberg uncertainty principle when using optical readout both in terms of intensity and phase measurements, which means that the lowest detectable concentration limits cannot be augmented beyond the current state of the art in classical sensors. Slight concentrations of trace gases, early indicators of failing mineshafts, or the first signs of vast reserves of oil, can be lost in the noise. However, the use of more general minimum uncertainty states in the form of squeezed light can push the noise floor in these sensors below the shot noise limit (SNL) in one analysis variable at the expense of another.

Reducing this noise floor is one of the major goals of quantum sensing research, and can be accomplished with several strategies: development of quantum light sources and detectors utilizing unique quantum properties such as entanglement and squeezing, and "quantum enhanced" optical fibers in which novel materials [i.e., nitrogen-vacancy (NV) centers] and/or structures are introduced specifically to interact with quantum light. Noise reduction can also be achieved in atomic sensors—devices which use populations of atoms rather than photons as the sensing field. These devices can serve as sub-SNL accelerometers, gravitometers, and interferometers in multiple sensing applications such oil and gas exploration.

3.1.1 Quantum Light Sources

The coherent-state uncertainty, or SNL, represents a minimum-uncertainty state[19]. Improvements in the SNL can be realized—to a point—by simply increasing the optical power of the platform's interrogation source. However, increasing power will result in signal saturation, heating, noise from parasitic nonlinear effects and, for fiber-optic sensors, will eventually result in damaged optical fiber.

It is possible, however, to reduce uncertainty in some quantum systems below the SNL without violating the Heisenberg uncertainty principle. In quantum noise reduction, or squeezing, the quantum statistics of a particular variable in a quantum system show reduced uncertainty compared to a coherent state[20]. States exhibiting quantum noise reduction (QNR) have reduced noise in one quadrature with respect to all states governed by classical statistics. The variables commonly associated with QNR in light fields are intensity and phase. It is possible to reduce the noise on one of the variables at the expense of noise on the conjugate variable using nonlinear optical interactions. With squeezing, the noise floor is reduced, and changes in the signal are easier to discern for the same confidence level or integration time.

Figure 2 shows the phase space for a coherent state and a squeezed state. Coherent states minimize the Heisenberg uncertainty principle with equal uncertainty in both quadratures as shown by the green uncertainty distribution. Squeezed states reduce the uncertainty in one quadrature while increasing uncertainty in the other as shown in blue. The first demonstration of squeezed light was obtained with four-wave mixing in sodium vapor[21], followed by many other atomic vapor experiments [22–28]. Optical parametric oscillators and amplifiers have also been used extensively to produce quantum noise reduction [29–32]. Four-wave mixing in atomic vapor does not involve optical cavities or interferometric control and can be integrated into a small package [33, 34].

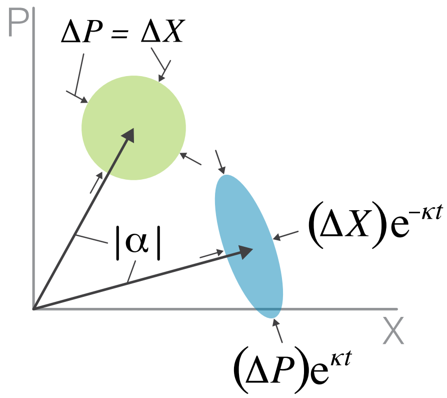


FIGURE 2. *Phase-space diagram showing the difference between a squeezed state (blue) and a coherent state (green). The shaded regions represent noise areas, the region in phase space in which a measurement would fall based on the uncertainty associated with the measured variable[21].*

It is clear that these squeezed light sources can lead to better signal to noise ratios for sensors that rely on measurements of the phase or amplitude of an optical readout. Perhaps the most well-known example of such a quantum sensor is the advanced LIGO platform for detection of gravitational waves [35], while other example prototype quantum sensors have enabled imaging[36, 37], magnetometry[38], atomic force microscopy[39], and plasmonic sensing[40, 41] of signatures that were previously obscured by quantum noise. Multiple proofs of principle have shown that squeezed light-based sensors can be integrated into compact packages for use in rugged applications.

Many quantum sensing approaches are also based on the availability of single photon sources and detectors. The investigation of the underlying photon correlations and statistics depends critically on the fidelity of the detectors. Specific examples include use of single photon detectors in fiber-based distributed sensing, a strong sensing system in fossil energy work. Avalanche-type photodetectors, superconducting nanowires, and photomultipliers are examples of systems with single-photon sensitivities that in combination with frequency counters and other electronic pulse processing systems can provide photon counting ability. Quantum sensing, more specifically, quantum optical sensing, requires use of single-photon detectors for experiments involving entangled photon pairs, photon anti-bunching, etc.

3.1.2 Sensing Applications

A major workhorse in the fossil energy industry is the fiber optic sensor. Fiber optic sensors, both distributed and single point, capitalize on fundamental photon-matter interactions to enable detection of external stimuli, such as temperature and pressure variations, in the medium in which the fiber is suspended. Of particular interest is the use of fiber optic sensors for oil and gas applications or geophysical research for carbon capture and storage. Both of these applications require that fiber sensors be deployed in harsh environments with temperatures in excess of 250°C and pressures several orders of magnitude greater than atmospheric pressure. Measurements of interest include dynamic and static strain, magnetic fields, temperature, and others. Limitations on the sensitivity of these measurements, and the subsequent bottlenecks in data analysis, place lower bounds on the accuracy and resolution of geological data collection.

These limitations are due to several factors, namely, (1) inherent limitations of the current laser sources; (2) inefficient and noisy optical detectors; (3) use of non-optimal optical fiber sensors; and (4) the brute force method of data collection. Advances over the current state of the art require efforts in these four areas, yet with today's technology rapidly approaching the fundamental limits imposed by classical (i.e., non-quantum) physics, improvements in sensor and sensing platform performance have slowed. Replacing the standard interrogating field with squeezed light would yield benefits in terms of SNR, but losses in the fiber could limit the gains somewhat.

Rare earth element detection is another key FE application. Near-distance standoff photo-absorption techniques in the visible (vis) and near infrared (near-IR) spectral regions offer a potential method for detecting rare earth elements, and these methods are compatible with squeezed light via quantum illumination [42]. These elements possess spectral signatures in the vis-near-IR that could be used in a detection attempt for standoff distances suitable for a drone. Development of portable standoff detection requires return photon signals of sufficient SNR. By employing the quantum properties in the photon statistics via quantum illumination, improved SNR may be achieved. Such an approach may overcome the current bottlenecks in satellite-based detection approaches.

Another interesting application involves gravity measurements via atomic clocks. Entangling a minimum of two atomic clocks that are geographically distant is expected to increase the accuracy of the clocks. Entangling an array of atomic clocks has been proposed to achieve shared timing information with an accuracy approaching the fundamental precision Heisenberg limit[43]. Therefore, sensors relying on time order, or sensors relying on ultrafast optics or dynamics can benefit from entangled atomic clocks. In general, sensors benefitting from a universal frame for time and frequency measurements will perform with more accuracy if entangled clocks can be distributed over geographically relevant sites for oil & gas exploration. Another example is better assessment of Earth's gravitational field and thus local density of earth—according to "relativistic geodesy," where gravity is measured at different locations on earth from measuring the rates of different clocks. Therefore, by invoking precision metrology afforded by the universal platform of time and frequency offered by entangled clocks, the frequency and amplitude of minute gravity oscillations associated with the breathing modes of earth may be detected. In mining, for example, ultrafast and ultraprecise detection of the extent of explosion and gravity fluctuations, stress variation (e.g., as a result of transient mechanical waves), presence of and displacement in fluids, etc., can prove useful in better design and control.

The applications above are only a small sample of a larger array of possible fossil energy applications for quantum sensing. In most cases, applicable quantum sensors could be brought to deployment within a few years. In the near term (0–3 years) we expect certain proof-of-principle laboratory-scale demonstrations to take place, in which squeezed light or entangled photons are used to enhance spectroscopy, standoff detection, and radar/lidar applications. Simultaneously, we expect advances to mitigate loss in fiber optic sensors that will make quantum fiber optic sensors viable in the medium (3–10 year) time frame. The most rigorous environments—well and subsurface applications—are expected to become feasible in the 10-year timeframe, though a combination of advances in quantum light sources, loss mitigation, and sensing protocols may move this timeline up considerably, by perhaps as much as 5 years.

3.2 Subsurface

3.2.1 Introduction

Subsurface systems host large reserves of fossil fuel, provide locations for long-term storage of energy by-products such as carbon dioxide, and may have roles for large-scale transient energy storage. Engineering uses of subsurface systems typically involve the injection and withdrawal of fluids in underground reservoirs, and successful operations rely on a robust understanding of the interactions among connate and injected fluids and minerals[44], as well as the ability to acquire and interpret changing signals of subsurface structure[45]. Quantum sensing approaches, particularly quantum magnetometry, offer a growing suite of new methods for physical metrology and chemical sensing[46]. Transferring these approaches to laboratory research and, ultimately, to field operations will offer opportunities to reduce the uncertainties in subsurface operations.

Magnetometry with quantum sensors uses the magnetic moment, or spin, possessed by electrons and some nuclei for highly sensitive measurements of static (DC) and time-varying (AC) magnetic fields[47]. Quantum-based DC vector magnetometers are able to measure the strength and direction of magnetic fields with the highest sensitivity currently possible[48] and have been translated to relatively mature commercial devices available for mapping small anomalies in the Earth's magnetic field for geoprospecting and navigation (e.g., as an alternative to GPS). Quantum sensor AC magnetometers can detect the small magnetic field fluctuations caused by the spin transitions of electrons and nuclei in their environment. They can serve as nanoscale reporters of the nuclear magnetic resonance (NMR) spectra of close-by molecules, providing access to powerful NMR characterization methods[49, 50]. In addition to sensing molecules, an exciting direction is the use of quantum magnetometers to coherently control the spin states of neighboring nuclei[51, 52]. Extending these methods to polarize the nuclei of fluid or solute molecules will realize dramatic signal enhancements for NMR and magnetic resonance imaging (MRI).

For a quantum system to function as a sensor it must possess energy-separated states and the ability to manipulate and read out which state(s) the system is in[53]. Environmental parameters can be detectable if they alter the quantum system in several ways. For example, quantum sensing can be performed if a field alters the energy spacings between states. Thus, a DC magnetic field is detectable when it alters the energy spacing for different orientations of the spin relative to the field. Quantum sensing can also be performed if the parameter changes the probability of finding the system in a different state after a period of time. For example, an AC magnetic field is detectable if the frequency, ω, is equal to a sensor spin transition energy and drives resonant changes in spin state. More usefully, non-resonant AC fields, including those for which the frequency is much less than spin transition energies, can be detected through their influence on the rate at which the system evolves between energy-separated or energy-equivalent (degenerate) states. The most sensitive approaches for NMR chemical quantum sensing use sequences that toggle spin-state transitions interspersed with free sensing steps. Such dynamic decoupling approaches protect the quantum sensor from environmental noise while measuring the analyte spin transition signal at or across the frequency range for the target nucleus.

Practical quantum sensing in the lab and field requires systems that exhibit quantum behavior at ambient temperatures and, to date, two technologies have met these requirements. Atomic vapor magnetometers generate clouds of alkali earth metals, such as Cs, K and Rb, and use laser light to excite an electronic transition that turns the vapor optically transparent with a high population of electrons in a spin sensing state. Interactions between the spins and an environmental magnetic field alter the population of the initial state and are detectable through changes in optical absorption. Typical vapor cells are ~10-mm dimensions although sub-millimeter-scale devices have been fabricated[54].

The negatively-charged nitrogen–vacancy (NV^-) center in diamond is an electronic spin-1 defect site formed by a nitrogen substitution adjacent to an empty lattice site[47, 55]. The ground state of this paramagnetic site has three spin states with energy separations that can be manipulated by a static magnetic field and energy transitions that can be driven with microwave radiation. The electronic properties of the NV^- center enable optical initiation into a single paramagnetic spin state and optical readout of the occupancy of the magnetic states through a change in fluorescence intensity.

Many physical and chemical sensing approaches have been demonstrated at the nanoscale using individual NV^- centers just within the surface of a single crystal diamond[56, 57] or the submicron scale using ensembles of NV[50]. Additional directions include functionalizing atomic force microscopy tips with NV^- centers[58], measuring stress distributions in high-pressure geologic research using diamond anvils[59], and using surface-functionalized diamond nanoparticles containing NV^- centers[60].

3.2.2 Laboratory Applications

The flow of a single fluid phase (such as water) through a microporous rock (such as sandstone) is well understood, but modern subsurface operations seek to flow or exchange multiple fluid phases and, increasingly, target nanoporous rocks such as unconventional shale reservoirs[61]. Moreover, there is growing interest in the use of complex fluid mixtures to adjust injectate viscosity, manipulate the rates of pressure and colloid transfer, and control subsurface chemistry. Diamond-based quantum sensing methods could be integrated into microfluidic devices developed for geoscience[62] to provide new insights into the interfacial molecular structure and macroscopic properties of common and novel fluids for subsurface operations.

3.2.3 Molecular Controls on Wetting and Multiphase Flow

Multiphase flow is very sensitive to the fluid–fluid and fluid–solid interactions that are quantified by wetting angles. For simple systems, molecular simulation can predict contact angles in good agreement with experiment (Fig. 3a)[63]. For multicomponent fluids, however, simulations predict that partitioning of molecules to interfaces can have strong effects on wetting angles, but no experimental approach has been able to perform spatially-resolved monolayer chemical speciation and simultaneous wetting-angle measurements. Integrating the diamond NV^- center into contact angle experiments (Fig. 3b)[49] could reveal the interactions between physical properties, such as molecular mobility (Fig. 3c)[49] and chemical composition[50] that lead to macroscale wetting behavior.

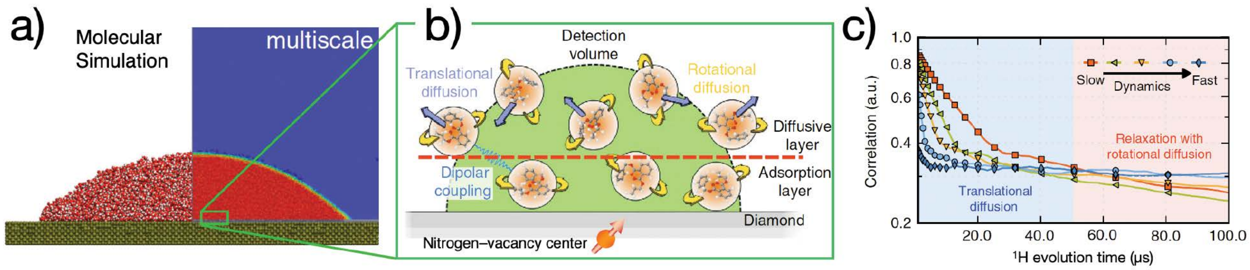


FIGURE 3. *Interfacial interactions controlling wetting angle. (a) Multiscale simulation of droplet spreading and contact angle prediction[63]. (b) Illustration of the use of a single NV^- site to monitor the molecular dynamics of oil molecules on a diamond surface[49]. (c) ^1H relaxometry obtained from the NV^- center shows that the molecules at the surface exhibit reduced mobility, and the translational and rotational diffusion varies differently as a function of the distance from the surface[49].*

Applications to subsurface settings will benefit from methods to modify diamond surface chemical properties through functionalization or the addition of inorganic coatings[60] and the study of multiphase fluids at relevant pressures and temperatures[64]. An exciting direction is the study of dynamic wetting in which molecular interface partitioning and the displacement of the contact line are highly coupled. A challenge will be the rapid acquisition of chemical information through the NV^- center, which will likely require the hyperpolarization method described below.

3.2.4 Rheology of CO_2 Foams

Supercritical carbon dioxide (sCO_2) has been extensively used for enhanced oil recovery in conventional and unconventional reservoirs, but the viscosity of sCO_2 is often too low for hydraulic fracturing applications. The rheological properties of sCO_2 can be manipulated by creating foams, energized fluids comprised of sCO_2 mixed with surfactants and, increasingly, with colloids[65]. Using surface functionalized nanodiamonds so that they partition into foam lamellae could enable local molecular properties to be determined in situ and correlated with macroscale flow (Figure 4). Quantum sensing with NV^- centers in nanodiamond is challenging because of a strong dependence of the signal on the orientation of the diamond lattice with respect to external magnetic fields. However, new quantum control methods are under development that allow orientations to be determined[66] or that could provide orientation independent sensing[67].

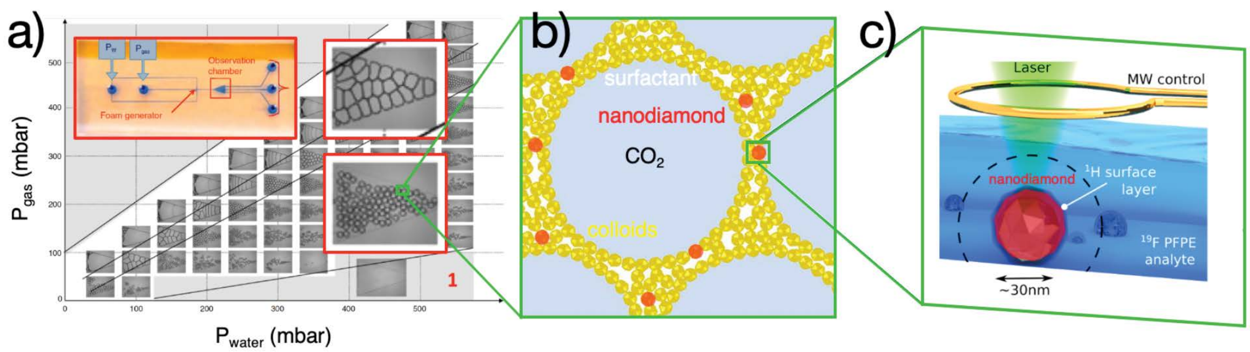


FIGURE 4. *Generation and analysis of foams for subsurface operations. (a) Foam structure regimes as a function of gas and fluid injection pressure can be visualized in a microfluidic device[68]. (b) Pickering emulsions are foams with stability enhanced by colloidal particles in the interfacial phase[69]. (c) The components of foam lamellae and local rheological properties could be monitored in situ using NV^- centers in nanodiamond[66].*

3.2.5 Optical Hyperpolarization of Fluids and Solutes

At room temperature and above, even in large magnetic fields, nuclear spins in fluid and solute molecules are distributed almost equally between opposite spin orientations, leading to small net signals in conventional and quantum magnetometry-based NMR and MRI. Approaches that polarize a larger fraction of the target nuclear spins than available at thermal equilibrium prior to measurement or imaging, called hyperpolarization, lead to dramatic enhancements in signal intensity. For example, ^{129}Xe nuclei can be optically hyperpolarized[70] and used to study transport in biological or microfluidic systems using MRI (Figure 5). A powerful approach under development is to use the electronic spins of NV^- centers to hyperpolarize target nuclei in the fluid or analyte of interest. Dynamic nuclear polarization (DNP) methods have been developed that transfer the NV^- spin polarization to ^{13}C nuclei in bulk crystal and nanocrystalline diamond and achieve orders of magnitude enhancement in the NMR signal[69]. The ability to routinely use NV^- based DNP to hyperpolarize external nuclei will dramatically reduce the time required to acquire physical and chemical data and introduce new applications such as measuring flow rates in porous media[71]. Because DNP requires relatively low power visible and microwave radiation, it can be integrated into microfluidics and, potentially, into field instrumentation.

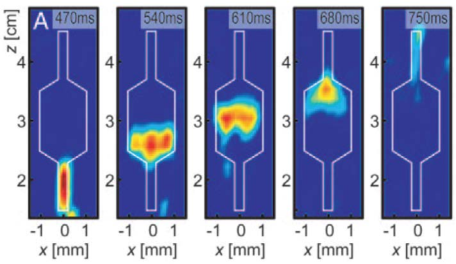


FIGURE 5. *Magnetic resonance imaging of hyperpolarized ^{129}Xe revealing fluid flow in a microfluidic channel*[70].

3.2.6 Field Applications

Although laboratory demonstrations of quantum sensing methodologies have to date been constructed on large optical benches[72], there is ample opportunity for miniaturizing the sensor, laser, microwave sources and control electronics, as well as rendering them compatible with relevant subsurface temperatures, such as temperatures above 150°C and hydrostatic pressures above 130 MPa.

3.2.7 Surface and Subsurface Chemical Analysis

The development of portable and economical quantum sensor technology and chemical spectroscopy to determine the composition of aqueous and non-aqueous fluids is likely to find application in many fields of the geosciences. Unlike conventional NMR instruments, which use high magnetic fields to discriminate between chemical species and boost signal, these new systems will require innovative approaches, currently underway, to detect molecules or characterize fluids in the low-field regime. For example, optical hyperpolarization transfer will enhance the signal at levels far greater than any superconducting magnet. Recently developed low-field detection schemes have demonstrated that full chemical analysis is possible at very low magnetic fields[73]. Ultimately, quantum sensors will offer compact approaches to characterize the viscosity and chemical constituents of injectate and produced fluids at the surface and deep underground.

3.2.8 Compact Borehole Porosity Logging

Characterizing porous rocks by quantifying the relaxation dynamics of proton spins of water or hydrocarbons has become an indispensable approach for distinguishing rock formations in borehole logging to optimize drilling and production[74]. Modern NMR logging tools use a permanent magnet to project a field into the formation and acquire spin relaxation and diffusion data to distinguish pore dimensions, estimate permeability, and determine water and hydrocarbon saturation states[75]. The ultra-high sensitivity of atomic magnetometers provides an opportunity to perform porosity characterization by detecting proton spin transitions in the Earth's magnetic field. At such low fields, the spin transitions can be detected at greater distances into the formation, providing a more statistically significant sampling and reducing the contributions from near-borehole processes that affected the earliest NMR logging tools. Laboratory studies have shown that atomic magnetometers can perform fluid identification at Earth field strengths[76].

3.3 Power Plant, Electrical Grid, and Oil & Gas Cybersecurity

In the near-term, researchers in quantum networking should attempt to learn from early industrial and commercial use of quantum key distribution (QKD) where valuable experience has been gained within pockets of industry attempting to utilize QKD. Such experience is essential in properly guiding QIS for practical quantum networking. In fact, research has failed to focus on some of the primary challenges of QKD (and by extension, quantum networking) in industry. For example, researchers are focused almost exclusively on faster key rate and quantum repeaters. While there is no doubt that faster key rate and longer distance are desirable features, more pressing issues for adoption are (1) lack of a common integration platform and standard for QKD with classical systems, (2) poor quantum scalability, (3) high cost, and perhaps most importantly, (4) lack of certification for QKD that is equivalent to that which is widely accepted for classical systems.

The most important near-term fossil energy goal should be to make fossil energy devices "quantum ready," not only for QKD but beyond, for general quantum communication and networking that provides benefits beyond cybersecurity. This goal includes integration with existing classical networks and standards such as, for example, General Electric's (GE's) Digital Ghost, and perhaps, more specifically, to quantum-secure sensors. A quantum internet with interconnecting quantum sensors is a suggested goal for the short- and mid-term.

(1) Continued cost reduction and (2) integrated quantum network security and sensing should be pursued in the mid-term. These goals include QKD and other quantum networking protocols implemented within a small form-factor inside grid, oil and gas, and other fossil energy rack-mounted devices as well as directly integrated on-chip. Having already established quantum-ready software and hardware as suggested for shorter-term goals, uptake of these mid-term goals will be more likely to occur within industry.

In the longer-term, lessons learned from QKD in industry are critical for extending the quantum channel into a quantum internet, whose base technology is likely to be entanglement distribution. This effort should be pursued for quantum-secure interconnectivity among processors, sensors, and legacy systems. The following subsections outline problems and potential solutions in more detail as seen from an industry perspective.

3.3.1 Short Term – Establishing a Quantum-Ready Base

Problem: The biggest challenge to power plant, electrical grid, and oil and gas pipeline cybersecurity is the ponderous investment in classical cybersecurity software, hardware, standards, certifications, and regulations that make it difficult to implement, test, or demonstrate quantum technology. A large suite of communication and network standards has been implemented and is costly to modify, resulting in inertia based upon approaches that rely upon computational complexity rather than physics. These legacy cybersecurity implementations, by definition, result in closed systems that are inaccessible to modification and experimentation. While it is relatively easy to design a new, stand-alone experimental quantum network, it is very challenging (often impossible) to incorporate such technology into a commercial system. Also, industry is unlikely to discontinuously switch to a quantum system. New technologies, including quantum technologies, rarely survive the cost of transition to a commercial product. All other technical challenges stem in whole or in part from this problem.

Solution: Planning the transition to a quantum network should be starting now. Flexible networks and standards will reduce the cost of integrating quantum technologies, making adoption faster and more likely. There are many lower-level quantum networking choices; for example, continuous-variable qumode transport vs. discrete-variable qubits as well as a variety of quantum protocols that could be implemented and tested. Software-defined Networking[77] and Active Networking[78] (Figure 6) are ideal classical solutions to enable flexible integration with quantum networking. Designing and testing flexible quantum network architectures should begin now rather than wait for the slow process of standardization later.

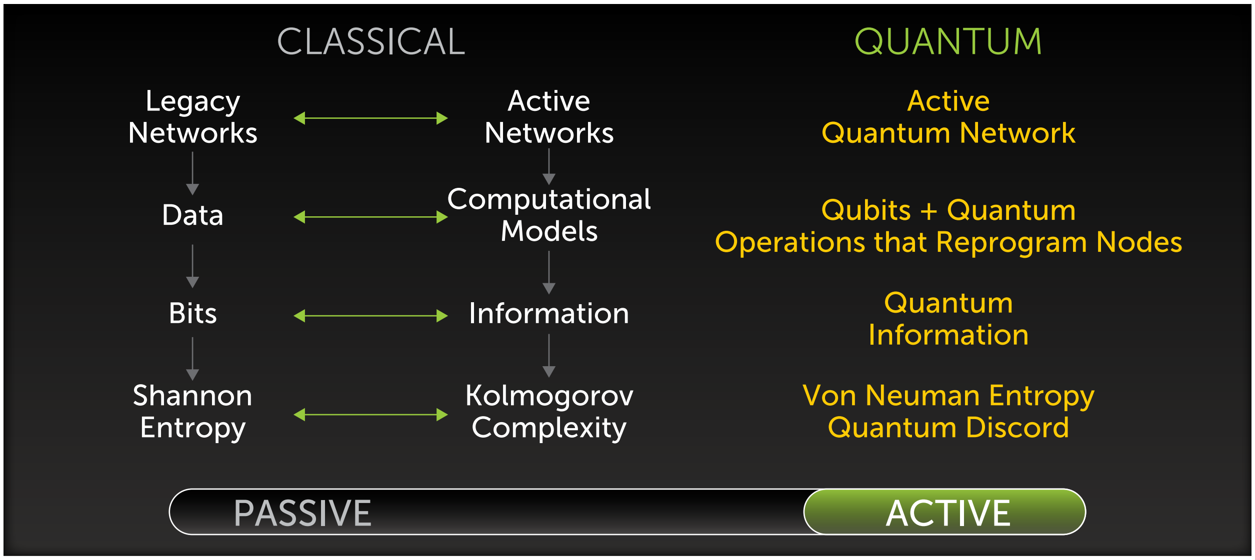


FIGURE 6. *Quantum active networks are hybrid classical-quantum active networks that enable the network to dynamically change its operation while traffic is flowing and where the traffic carries the instructions to change the network. Thus, the network becomes a hybrid quantum transport and computing system, enabling rapid exploration of new ideas that benefit both networking and computation*[78].

3.3.2 Short-Term – Establishing Quantum-Ready Fossil Energy Communication Systems

Problem: Commercial QKD systems are emerging and creating software, hardware, and standards of their own. However, they are struggling against the titanic legacy investment in classical security, including the touted benefit of post-quantum cryptography, which claims to solve security against a quantum computer for free without requiring quantum hardware. Quantum technology must demonstrate not only that it is better than classical, but also that it is many orders of magnitude better in order to be considered for adoption. The problem is how to best leverage the small, early successes of QKD for more general quantum communication and networks when there is uncertainty in how quantum technology will evolve or be certified. The transition to QKD and quantum networking is expensive and will require demonstrating more value than simply providing cybersecurity, whose value is notoriously difficult to quantify. A quantum network can demonstrate more value over classical networks by performing quantum sensing and computation in addition to cybersecurity.

Solution: Develop flexible networks and standards for integration with quantum sensing and computation. Benchmarks that clearly define quantum metrics vs. classical should be defined for QKD, networking, and sensing, and means of quantum cybersecurity certification need to be developed now. Networking architectures that best handle quantum interfaces, i.e., quantum transduction, should be considered. Networks that anticipate a variety of quantum technologies, including entanglement distribution as a generic service, should begin to be built. Management and control of quantum networks needs to be considered now. Integration with existing communication and networks will be a requirement for industry. We need to begin extending industrial networks and cybersecurity, e.g., GE's Digital Ghost, toward quantum networks for adoption of any quantum technology. We should be anticipating the flexibility required for future quantum technologies now. But there is a chicken-and-egg problem, industry will not invest in such things until quantum technologies achieve some form of a security certification or regulatory requirement.

3.3.3 Short-Term – Generating Quantum (QKD) "Pull" from the Customer

Problem: A perceived problem is the knowledge/awareness gap between QKD technology expertise, domain-specific expertise in the field of power generation and distribution, and the joint application of both. Power generation and distribution domain expertise is often characterized by individuals having a minimum of two decades in the field with significant practical experience. As QKD technology evolves from research, a significant gap between the lab and practical implementation exists. There is no "pull" from industrial users for a quantum technology, thus vendors have no realistic incentive to implement it. This problem is due to a lack of benchmarks and certification.

Solution: Identify a target system/use case that utilizes conventional cybersecurity technologies, map it out, overlay it with current QKD techniques, and map out the entire life-cycle from design, implementation, configuration, operation, and maintenance to highlight those areas of focus that will enable the adoption of QKD technologies as identified by non-QKD experts who are more knowledgeable in the domains of energy, transmission, and distribution and other fossil energy networks and who can provide valuable input to government certification authorities.

3.3.4 Short-Term – Quantum Trusted Platform Integration

Problem: Fossil energy systems rely upon variants of classical cybersecurity (e.g., trusted platform modules [TPM]). TPMs, in turn, rely upon asymmetric public key cryptography for their security and are also cryptographically tied to the configuration of a specific device—either a computational platform or a sensor. TPMs are thus subject to quantum computing and other attacks, and if relied upon to protect sensors in the power grid (as they are now), are susceptible to manipulation to inject false readings and cause significant damage.

Solution: Development of a quantum TPM, in which the full benefit of QKD is used to protect a device, would further test, expand, and demonstrate the benefits of quantum security. Researching the feasibility of a quantum TPM is of immediate use in industry.

3.3.5 Short-Term – Cost and Reliability

Problem: The rate of adoption of quantum technology will increase as cost is reduced. Classical cybersecurity is so ingrained within industry that it is often touted as free and without overhead. While this is untrue, quantum cybersecurity will be forced to reduce cost by many orders of magnitude to become equally viable.

Solution: The cost of single-photon sources and detectors, both bulk and within integrated optical chip solutions, will need to be reduced. Another key requirement is room temperature (or near-real-time) operation of such devices and their ability to survive the harsh environments found in many oil and gas applications.

3.3.6 Short-Term – Tighter integration of Classical and Quantum Networks

Problem: Quantum technologies added as optional overlays, as many are now, are less secure and efficient than if they were integrated with the powerplant, electrical grid, or oil and gas pipeline software/hardware infrastructure. QKD integrated within its target devices is less susceptible to attack.

Solution: Tighter integration of QKD and quantum communication with the powerplant, electrical grid, and oil and gas pipeline will increase security and reduce cost. Integrated QKD and integrated quantum communication chips as well as integrated fiber-optic sensors offer promise. Quantum fiber optic sensing has evolved from a research topic to a real-life industrial application with a range of functions. Fiber optic distributed sensors can be used for monitoring temperature distributions along power cables to optimize current-carrying capacity, in subsea oil pipelines for flow assurance, and along gas pipelines to detect high-pressure leaks. Their use is also becoming common in structural monitoring applications for civil structures such as bridges and dams, as well as pipelines in unstable geotechnical regions. Research into enhancing these sensors with quantum capability could yield significant benefit.

3.3.7 Short-Term – Quantum Network Scalability

Problem: Quantum technologies, whether qubits, secret-sharing partners, or sensors are currently not directly scalable to the magnitude required by industry.

Solution: A quantum communication network architecture that compensates for lack of scalability could enhance adoption of the technology by industry. Again, this goes back to the importance of defining a flexible, quantum-ready network architecture.

3.3.8 Short-Term – QKD and Quantum Communication Certification

Problem: The industry is understandably reluctant to accept risk. The lack of regulatory requirements and certification for quantum technology, e.g., quantum random number generation (QRNG) and QKD make adoption by industry difficult, if not impossible.

Solution: Projects that lead to determining the essence of QRNG and QKD regulatory requirements and certification would greatly benefit industry. These projects could be performed in collaboration with agencies like NIST or MITRE. A broad study and taxonomy of QKD protocols and their integration with classical cybersecurity might be useful in this regard.

3.3.9 Short-Term – Quantum Secure Time Synchronization

Problem: Industrial systems require real-time control, and thus secure and stable time synchronization. As classical communication becomes faster, higher resolution time synchronization is required and the corresponding time stability requirements increase.

Solution: Protocols for quantum-secure time synchronization would be desirable. Quantum entanglement of clocks is one possible solution, ideally in collaboration with NIST. As previously mentioned, a flexible, quantum-ready network architecture will greatly facilitate adoption.

3.3.10 Medium-Term – Untethered Quantum Communication

Problem: The current media for commercial QKD requires a fiber quantum channel. This adds cost and restricts movement. However, space-based quantum systems are far too expensive and overkill for industrial use. A terrestrial untethered quantum communication medium will be needed.

Solution: A secure 5G or Wi-Fi equivalent for wireless quantum communication (WQC) or wireless QKD (WQKD) would be an ideal solution. Microwave QKD is a step in this direction; however, a radio frequency-like solution would be ideal. Research on this topic is needed for industrial environments.

3.3.11 Medium-Term – Quantum Distance Limitation

Problem: Attaining the full benefit of quantum cybersecurity could require a quantum channel the length of the diameter of the network, i.e., along its backbone. While space-based systems can extend further than terrestrial networks, terrestrial quantum channels are currently limited to approximately 420 km. Extending the length of terrestrial quantum channels is needed to reduce dependence upon "trusted" relays (which we realize is a euphemism for vulnerable relays).

Solution: The use of quantum repeaters to extend the distance of terrestrial quantum networks is one solution. The approaches being explored to develop quantum repeaters will also enable a fully quantum internet.

3.3.12 Long-Term – Quantum Transduction

Problem: Quantum systems comprised of disparate technologies and operating at different frequencies require interconnectivity. For example, quantum processors and sensors would benefit from secure interconnectivity over the same quantum network.

Solution: Quantum transducers convert quantum signals from one form of energy to another, enabling quantum information to be seamlessly conveyed among devices on a quantum network. More research in this area is needed.

3.3.13 Long-Term – Quantum Secure Sensors and Quantum Sensor Networking: Quantum Industrial Internet of Things

Problem: The danger of compromised sensors is a well-known problem in industrial applications. Maliciously created false readings can cause life-threatening situations.

Solution: Extending quantum security to sensors, and in the longer-term, to quantum sensors that inherently transport results over the quantum network as quantum state, are possible solutions to explore.

3.3.14 Collaboration for Quantum Network Standardization

Industry collaboration for the standards development process is required. The Quantum Economic Development Consortium[79] has found that quantum communication and networking is leading all quantum technologies in standards development via a variety of standards development organizations, including the Internet Engineering Task Force, International Telecommunication Union, European Telecommunications Standards Institute, IEEE, and others. Support for the development of quality quantum networking standards that enable vendors to mix-and-match as well as easily integrate new quantum software and hardware is required for adoption by industry. DOE's help in this regard would greatly advance adoption and commercial sustainability of quantum technology.

3.3.15 Recommendation

Most of the solutions outlined in this section lead to the conclusion that a flexible, extensible quantum-ready network architecture for fossil energy—one that can operate with quantum systems through common management and control—is needed now. Such a system should demonstrate classical sensors protected by QKD as well as new quantum sensing mechanisms for all fossil energy industries.

3.4 Materials Development

In the real world, almost everything can benefit from quantum computing with exponential speed-up. The use of quantum computation in material sciences is rapidly growing as quantum computers become more technologically mature[80–82]. Among digital and analog quantum simulations, analog simulation is better for larger systems, especially for designing materials. To achieve effective quantum simulation, the variational algorithms that utilize hybrid approaches where both the quantum and classical computer are working in tandem are becoming useful, as such algorithms partly avoid the shortcomings of current hardware limitations in quantum computers. Such computational approaches are known as hybrid quantum-classical algorithms, and these are more practical frameworks for simulating heuristics models in noisy intermediate-scale quantum. In order to solve classically intractable quantum chemistry problems with a quantum computer, the first step is the state preparation. In the seminal work of Zalka[83], discretizing the wave function and initializing the simulation using a series of controlled reactions was proposed. Conceptually, discretizing a many-body Hamiltonian using the second quantization while preparing the quantum states, which will eventually be formulated in terms of qubits, is easier and less mathematically involved [84–86].

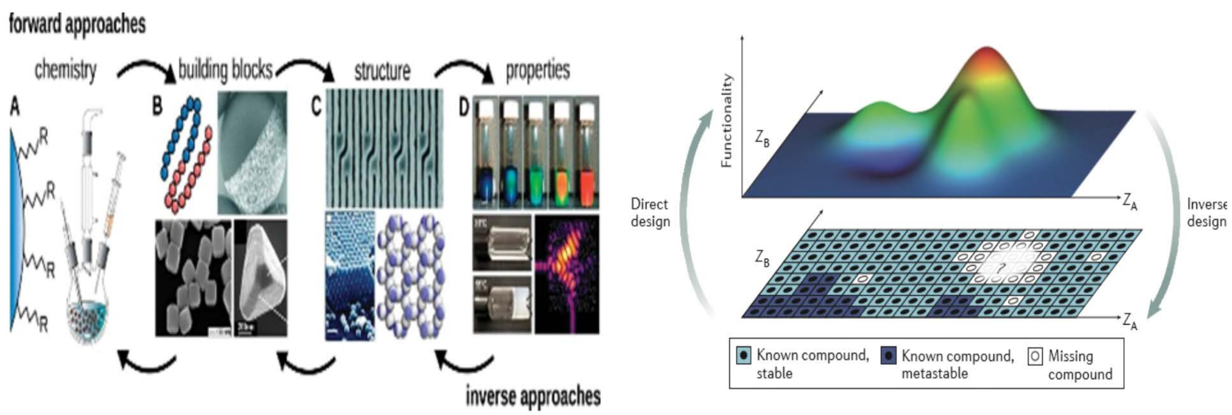
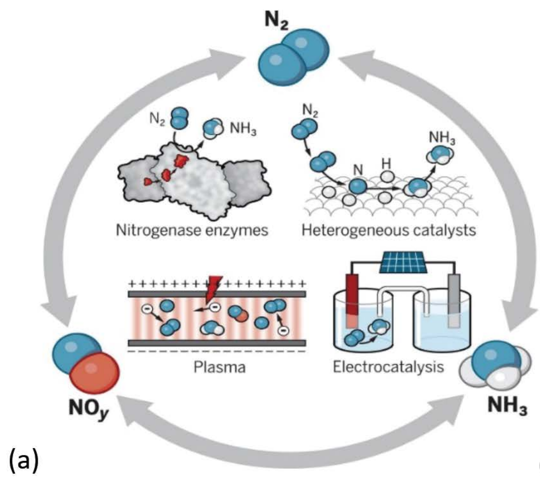


FIGURE 7. *Forward and inverse approaches in discovery and design of materials. (left) Materials with new properties may be discovered by repeatedly carrying out the following sequence of steps[87]. (right) In functionality-directed material discovery or inverse design, only those compounds with the target (or maximal) functionality are investigated[88].*

Generally, the *Forward* strategies for discovering new self-assembling materials are commonly adopted. In such approaches, an initial set of material building blocks is synthesized, and protocols are chosen to promote their self-assembly in an experiment or a computer simulation. The structure and properties of the resulting material are subsequently characterized. However, recent research indicated that formulating such a process as an inverse problem can be helpful in making materials discovery more systematic and amenable to meeting specified design constraints. For example, in Figure 7 (left), Sherman et al[87] defined a figure of merit based on a desired structure or macroscopic property and then applied methods of constrained optimization to help navigate the multidimensional design space and determine which available building blocks, interactions, or protocols are most suitable for realizing a material. Solid-state chemists have been consistently successful in envisioning and making new materials, often enlisting the tools of theoretical solid-state physics to explain some of the observed properties of the new materials. Based on the Periodic Table and the proposed properties, with applying inverse design as demonstrated in Figure 7 (right), Zunger et al[88-91] illustrated a new style of collaboration between theory and experiment via an inverse approach to design new materials that have not yet been synthesized. Recently, machine learning (ML) has been applied to materials development. Many new materials have been computationally synthesized by combining ML with inverse design (i.e., photonic and photovoltaic materials [92-94], A_2BX_4-type metal-chalcogenide compounds[95, 96], low-battery materials[97], Metal Organics Frameworks (MOFs) and membranes for gas separations[98, 99], etc.).

Rapid recent advances in quantum technology have enabled quantum computers to be used to elucidate reaction mechanisms in complex chemical systems. Figure 8(a) shows possible routes for nitrogen transformations[100]. Among them, the biological conversion uses an enzyme (nitrogenase) to catalyze the conversion of atmospheric nitrogen molecules into ammonia through a process known as nitrogen fixation. Figure 8(b) shows a flowchart for a hybrid type of calculation where a quantum computer augments a classical computer in the calculation of the classically intractable problem of correlation energy under complete active orbital space[80]. Reiher et al[80] used this scheme to show the resource requirements, including error correction, for the simulations of the cofactor FeMoco of nitrogenase using quantum logic gates operating at 100 MHz with an error target of 0.1 milli Hartree. These results indicate that the necessary computations can be performed in a reasonable time on small quantum computers, which are able to tackle important problems in chemistry without exorbitant resources[80, 101]. Such a hybrid classical-quantum computer approach can be used for calculating other complex systems.



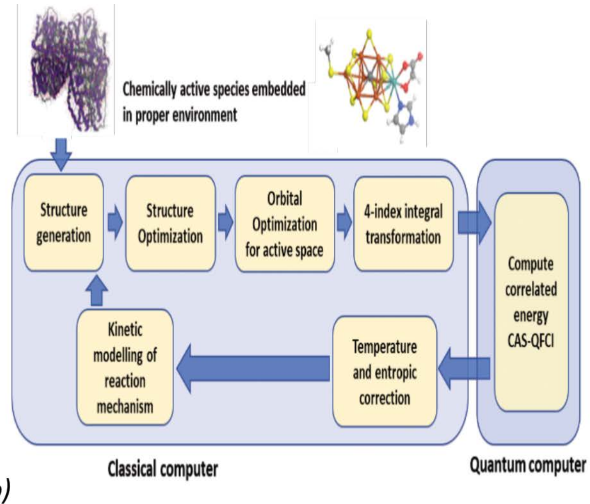


FIGURE 8. *(a) Possible routes for nitrogen transformation*[100]*; (b) Generic flowchart of a computational reaction mechanism elucidation with a quantum computer part that delivers a quantum full configuration interaction energy in a (restricted) complete active orbital space*[80].

Designing new catalysts and exploring novel catalytic reactions are key challenges for the Materials community. First principles-based molecular modeling plays a crucial role in the development of novel catalytic materials and the investigation of catalytic chemical reactions. However, the computational cost and/or the accuracy of these models remains a bottleneck in carrying out these simulations for complex or large-scale systems, as in the case of catalysis. Over the past two decades, ML has made an impact on the field of computational catalysis. Researchers have started using ML-based data-driven techniques to overcome the limitations of these molecular simulations[102, 103]. Obviously, quantum computing can speed up such molecular simulations for materials development. The following sections illustrate several possible directions to develop materials for fossil energy related applications.

3.4.1 Game-changing catalysts for direct methane conversion

The conversion of methane (CH_4) into an easily transportable liquid fuel (e.g., CH_3OH) or chemicals has become a highly sought-after goal spurred by the increasing availability of cheap and abundant natural gas. While utilization of methane for the production of syngas and its subsequent conversion via an indirect route is typical, it is cost-intensive. Thus, recently, alternative direct conversion routes have been actively investigated. One of the most promising routes is the low-temperature partial oxidation of methane to methanol over a metal-loaded zeolite, which mimics facile enzymatic chemistry of methane oxidation[104, 105]. Currently, the most important catalyst for CH_4 conversion is $Cu/ZnO/Al_2O_3$ and Cu-zeolites. Copper is also an excellent Water-Gas Shift catalyst facilitating the conversion of CO to CO_2 and vice versa. While controversy about the carbon source in methanol synthesis still present, most researchers are in favor of CO_2 hydrogenation mechanisms (Figure 9 (a)) [105]. Obviously, catalysis for methane conversion to methanol is low-hanging fruit for catalyst design and quantum computing. Identifying these materials and step-changing catalysts would be game changing.

3.4.2 Multi-metallic oxygen carriers for chemical looping process

Chemical looping combustion (CLC) is a cutting-edge combustion technology that enables CO_2 capture without a major energy penalty in separation. The technology involves the use of solid metal oxides, so-called oxygen carriers, which are alternately subjected to redox reactions[106]. In recent years, most investigations of the CLC process have been focused on the development of synthetic multi-metallic oxygen carriers, which are much more efficient and have greater resistance compared to natural materials. Although chemical looping beyond combustion (CLBC) has attracted increasing attention over the past 5–10 years, this emerging research area is far from being adequately explored, particularly considering its significant complexity and excellent potential as demonstrated in Figure 9(b)[107]. Redox catalysts can undergo significant changes to their surface and bulk properties within a CLBC cycle that exceeds the complexities typically observed in heterogeneous catalysts. Such complexities should be addressed through continued research via interdisciplinary efforts and aided by quantum computations.

3.4.3 Materials for carbon capture and utilization

The role of carbon emissions in climate change presents a significant environmental challenge, which requires more efficient materials to capture CO_2 from coal combustion and/or directly from air and to convert CO_2 into valuable products[108 – 110]. The concept of quantum algorithms can be readily applied to ML approaches for developing carbon capture technologies[111]. High-throughput screening of promising CO_2 capture materials from existing complex chemical compounds (such as solids, solvents, MOFs, matrix membranes, etc.) and theoretically designing new CO_2 capture materials have demonstrated success in improving the development of CO_2 capture technologies[99, 112]. As shown in Figure 9(c), Anderson et al.[113] implemented a multiscale approach by combining DFT, grand canonical Monte Carlo, and ML to investigate the role of various pore chemical and topological features in enhancing the CO_2 capture metrics of MOF materials. Algorithms based on quantum computation can avoid statistical complexity and can access a wider computational space, which enables a higher number of permutations and combinations during the materials screening and design process. In addition, such an approach with inverse design can be a powerful computational tool to design new catalysts for CO_2 conversion.

3.4.4 Advanced materials for energy storage

Development of next-generation energy storage materials is one of the hottest research topics in the materials science field. These materials can be used for H_2 storage, rechargeable secondary batteries, redox-flow batteries, supercapacitors, etc., to store chemical, thermal, or electrical energy[114–118]. Hybrid analog and digital simulations are powerful tools with which to tackle such materials development. Figure 9(d) shows an inverse design with generative deep learning for electrolyte materials development[119].

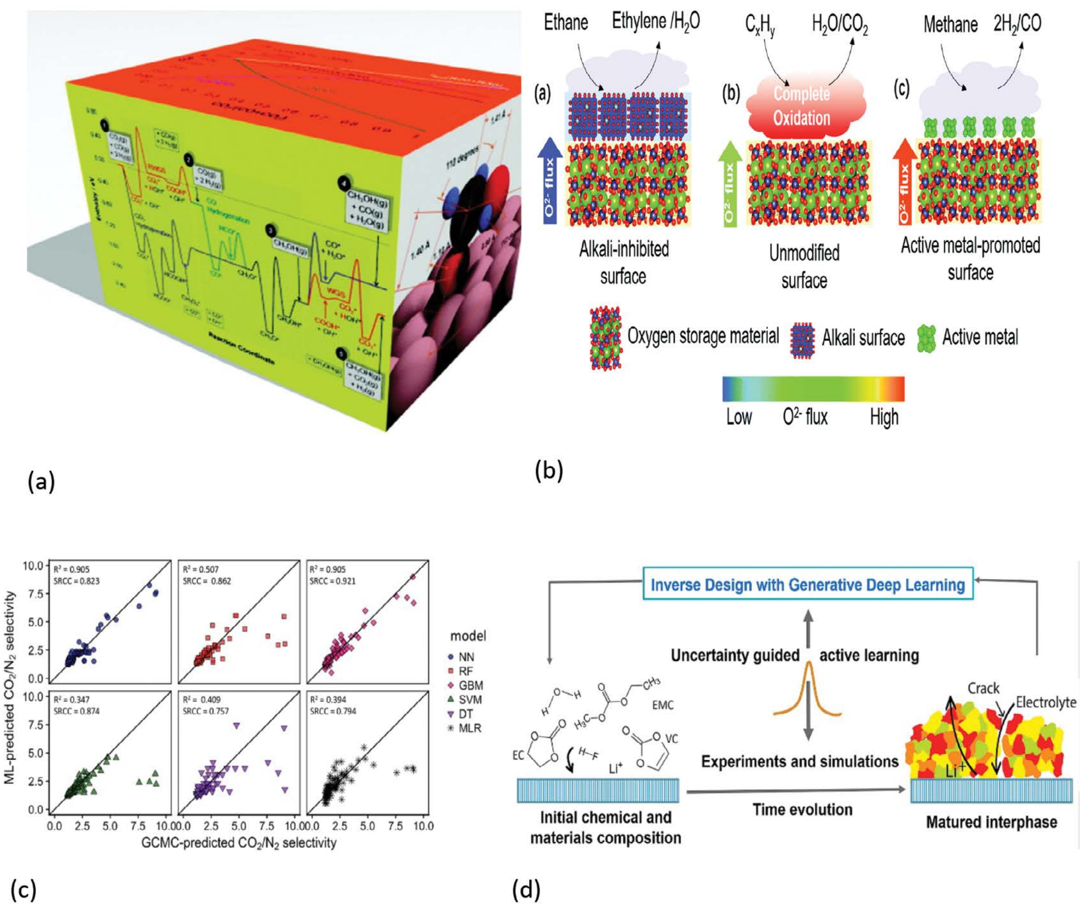


FIGURE 9. *(a) Convert CH_4/CO_2 into CH_3OH[102]; (b) Schematic illustration of surface modifications of redox catalysts to improve product selectivity by changing the relative rates of surface oxygen removal and bulk O_2 – flux. The arrows in the three cases (a–c) correspond to the O_2 – fluxes and the colors correspond to the relative intensity of the O_2 – fluxes[107]; (c) Parity plots comparing the prediction of CO_2 selectivity over N_2 by various trained machine learning algorithms versus the prediction from Grand Canonical Monte Carlo (GCMC) molecular simulations on the test set[113]; (d) Inverse electrolyte design with generative deep learning[119].*

3.4.5 Recommendations

The discovery of materials with specific properties has been slow and difficult to accomplish. The ability to computationally identify materials is proving to be a game changer (see example[99] on carbon capture). Quantum mechanical calculations are now helping us unravel previously unreported properties of synthesized materials. Many compounds that have never been synthesized appear to be chemically plausible. Catalysis for methane conversion to methanol, for example, is low hanging fruit for catalyst design. Materials for effective CO_2 capture and utilization is another example. Other materials of interest include those with self-healing abilities, tolerance of and resistance to environmental exposure, hydrophobicity, self-assembly capability, harnessing solar energy, etc.

- In the near-term, analog quantum simulators need to be explored for materials development because they are easier to construct in comparison with digital simulators.
- Catalyst design requires massive quantum computations; quantum ML algorithms for accelerating this type of materials development need to be developed.
- Inverse design for designing and synthesizing functional materials with proper properties for specific applications is an important area of research. Quantum computational algorithms for the inverse design of materials need to be developed.

3.5 Power Plant Design and Optimization

Research to design and optimize fossil energy systems to ensure a reliable and resilient U.S. bulk power system is increasing in importance. For example, advanced computational methods are being used to improve the operation of the existing fleet and to design new fossil energy systems, including hybrid systems that are optimized to dynamically interact with the emerging grid. As the size and complexity of the design space continues to grow, new computational approaches that can help solve the resulting multi-scale, nonlinear, dynamic optimization problems while accounting for multiple sources of uncertainty are needed.

Many optimization problems related to fossil energy systems are formulated as mixed integer nonlinear problems (MINLP), which are non-deterministic polynomial-time hard (NP-hard). While current algorithms can solve many problems to global optimality (Figure 10), more than 30% of test problems still cannot be solved.

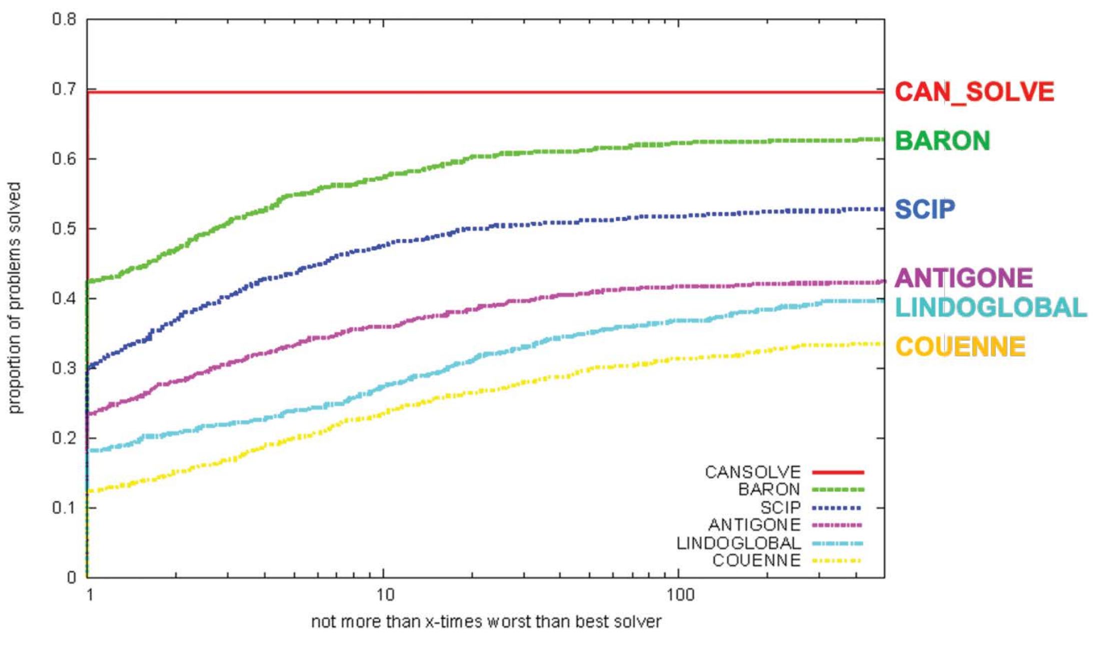


FIGURE 10. *Comparisons based on solver ability to prove global optimality*[120]

This gap represents a near-term opportunity for quantum computing to address fossil energy problems at multiple scales from molecular design[121], thermodynamics[122] and reactivity, conceptual design[123], process optimization[124], and energy infrastructure planning[125]. Recent trends are increasing the computational complexity associated with designing the fossil energy systems of the future. These include the need to design systems that are inherently dynamic and flexible. Understanding the requirements for flexibility requires integration with grid and dispatch models, which are themselves optimization problems. In addition, these grid models are region-dependent and are rapidly evolving, resulting in the need to solve a multi-scale MINLP under uncertainty. Another recent trend is to utilize process intensification to reduce costs and improve efficiency[126]. Such approaches require the ability to explore design spaces beyond current experience, often resulting in large-scale superstructure-based optimization problems. In addition, addressing such design problems may require scale-bridging techniques to integrate system design with device-scale design and optimization.

Various approaches for representing uncertainty in fossil energy systems have been utilized; however, solving the resulting optimization problems is challenging due to the increased computational complexity. Bayesian approaches have been demonstrated to provide a good way to represent uncertainty. Quantum computing techniques may enable new sampling approaches that could improve the efficiency of solving large-scale problems that include uncertainty. Some representations are more suitable for quantum computing than others. For example, the native problem representation for existing adiabatic (annealing) quantum computing technologies is a "quadratic unconstrained binary optimization" problem. The challenge for powerplant design and optimization is that the native superstructure models are highly constrained and include continuous variables. Unfortunately, current quantum algorithms for general optimization problems (e.g., based on Grover's search) do not promise significant scaling improvements over their classical counterparts. A promising area of research involves developing hybrid quantum/classical algorithms.

Quantum simulations have been demonstrated for Monte Carlo or stochastic simulations. Recently, hybrid classical-quantum algorithms have been demonstrated for modeling atomic-level chemistry. Such methods have used quantum computing approaches to optimize the "difficult" parts of molecular interactions. Opportunities to exploit this structure in the design of materials based on desired properties for a given application exist, thus enabling truly simultaneous design of materials and processes. In the near term, quantum annealing approaches may provide an opportunity to help address such large-scale optimization problems.

3.5.1 Recommendations

While it is clear that quantum computing could potentially help address challenges related to the design and optimization of fossil energy systems, a better understanding of both the potential benefits and challenges is needed. Among the challenges is determining how to effectively map problems/data into quantum compatible forms and back to classical formulations to enable hybrid computing approaches. An exploratory research project among fossil energy optimization experts and quantum information scientists to develop effective mapping approaches for problems/data into quantum compatible forms and back to classical formulations would enable an interface between classical and quantum computing that could be used to rapidly demonstrate potential benefits of quantum computing on ongoing fossil energy systems optimization priorities.

3.6 Power Plant Operation and Control

Fossil-fueled boilers used throughout the power generation industry emit various chemical compounds that must be tightly controlled for environmental purposes. The quantities of emissions of nitrogen and sulfur oxides (NOx, SOx), carbon monoxide (CO), and carbon dioxide (CO_2) are directly proportional to the amount of air and fuel that are mixed prior to combustion. The amount of excess air required to optimize safety and reliability while approaching complete combustion has approached optimal limits for coal-fired boilers but can be much higher during ever-increasing cycling operations (at lower loads). Some potential areas for quantum computing research (which will require substantial progress in quantum computer capabilities) that could address emissions include the following:

- Quantum-enabled excess air minimization: Fuel/air ratio optimization using real-time feedforward function block that derives actual excess O_2 from various downstream measurements combined with advanced chemistry modeling (real-time).
- Optimized environmental equipment control: NOx and SOx equipment (such as selective catalytic reduction and scrubbers) operation using advanced chemistry models (real-time).
- Improved burner design: The burner is the device in which the fuel/air mixture is introduced to the furnace section of the boiler. The burner design might be improved if new advanced chemistry model(s) are produced using quantum modeling.

Fossil-fueled boilers also must optimize operation while considering reliability of key components, most notably boiler tubes that continue to be the largest contributor to reliability issues. Boiler tube failure mechanisms are complex and involve an intersection of materials/chemistry and thermodynamics/heat transfer phenomena that is difficult to control during operation. Variables that limit the ability to optimize boiler tube reliability include fuel variability (e.g., different fuel compositions that are difficult to measure in real-time), deposits on and erosion of boiler tube surfaces, thermal stresses due to many factors including cycling operation, and complex heat transfer phenomena (combined conduction, convection, and radiation effects). Some potential research areas for quantum computing that can address reliability include the following:

- Improved data fidelity: Data from the various process instruments (temperature, flow, pressure, strain, etc.) are stored on hard drives that would fill up quickly if all dynamic conditions were recorded.
- Boiler component failure prediction: By using high-fidelity data and having an enhanced understanding of real-time materials/chemistry and thermodynamics/heat transfer phenomena, it might be possible to update boiler component (e.g., tubes) life predictions based on actual measurements.

The ability to collect and analyze real-time data combined with the ability to model the complex materials/chemistry and thermodynamics/heat transfer phenomena is at the core of enabling advancements in emissions reduction and improvements in component reliability. Boiler controls, combined with data/analytics, could be used in new ways to improve plant operations to meet emissions reduction targets while improving component reliability.

3.6.1 Recommendation

Improvements in process control and operation of fossil-fueled power plants are limited largely due to a lack of high-quality dynamic data. The past several decades of operation have proven that understanding and measuring degradation mechanisms and process parameters enables design and retrofit improvements, optimizes process control, and enhances reliability. Process sensors such as pressure, temperature, and flow have been used in combination with advanced regulatory controls—feedforward, cascade, gain scheduling, ratio control—to improve operation and reliability targets.

However, the data collected from process parameters are often stored in data historians with time records of one minute or more between samples. For example, a main steam temperature process parameter might be stored as 1050 degrees Fahrenheit (°F) at timestamp 2/2/2020 11:59:00 AM EST. The parameter at timestamp 2/2/2020 11:59:01 AM EST, unless greater than a 0.5°F change, might be stored as 1050°F when in-fact, the parameter might have been 1050.4°F when measured. When considering the dynamic conditions across the entire plant cycle, this practice of "data compression" effectively loses the ability to assess historical operations at the fidelity at which dynamic conditions are captured. This is important for two reasons: (1) process control optimization is limited to a macro understanding of dynamic behavior and (2) equipment reliability programs are based on overall thresholds on parameters instead of actual process dynamics.

As an example of the effects data compression have on data fidelity, consider Figure 11. On the left example, main steam temperature in blue is plotted versus compressed main steam temperature (stored) in orange. Intervals along the orange line that do not change illustrate a loss of data fidelity. On the right example, final feedwater temperature is subtracted from main steam temperature. The blue line is the uncompressed results and the orange line is the compressed results. There is at least a 1.2°F difference between the two in the area highlighted.

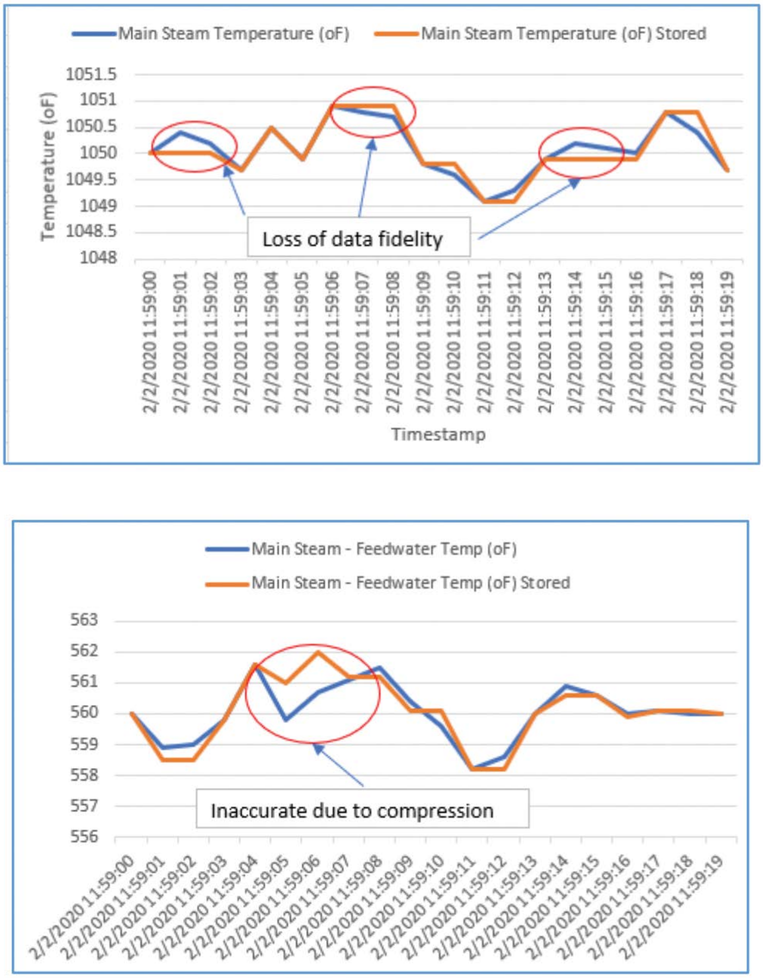


FIGURE 11. *Main Steam Temperature Data Compression (Left); Main Steam Temperature minus Final Feedwater Temperature (Right) (Original graphs created by author for this report.)*

Better data compression algorithms are needed in order to collect and store data under truly dynamic conditions in plant data historians. It would be impractical to store all data at high frequency (e.g., storing every 0.001°F of main steam temperature every 1 millisecond). Compression of thousands of process parameters is necessary due to the vast quantity of data—data stored every 1 millisecond for 1,000 parameters would quickly fill even the largest data archive systems that we have today.

Instead, it would be prudent to store only data for which process dynamics are changing when compared to historical values. This objective could be achieved by using machine learning (ML) to compare a vector quantity composed of individual process parameter measurements to an historical database of vectors to determine if there are truly any significant dynamics that should be archived. For example, consider Figure 12 as a concept. The blue vectors represent historical records that are stored in a data historian. Given many process variables, the vector dimensions might be on the order of 100 or even 1000, but the two-dimensional representation is easy to visualize. The black vector represents an incoming set of process parameter values. For example, the vector might represent final feedwater temperature and main steam temperature. The ML technique would compare the vector similarity to determine if the incoming vector is significantly different and, if so, the vector would be stored.

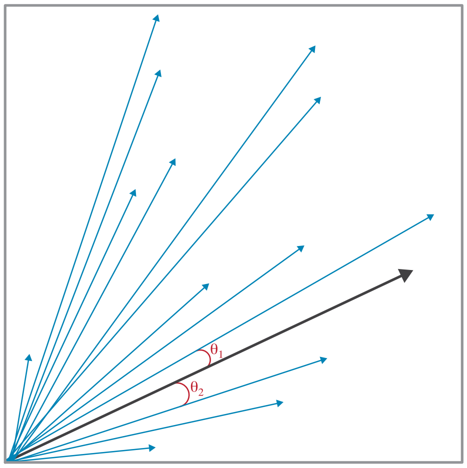


FIGURE 12. *Vector similarity to compare incoming data against historical records (Original graph created by author for this report.)*

The remaining challenge is to compare an incoming vector quantity to a large historical database of vectors at a processing frequency of at least 10 times that of the process parameter measurements. For example, if data might be stored at up to one millisecond intervals, the processing of the ML technique (to compare vectors) might need to occur at 100 nanoseconds.

Quantum algorithms might be able to process a vector (translated to quantum-space) against known vectors at the processing speed required (100 nanoseconds). The measured vector would need to be converted to a quantum vector at the input by a traditional computer then converted back to a traditional vector by the quantum computer “quantum data transform algorithm.” If these algorithms were able to run alongside traditional control systems, data measured and stored would have the fidelity necessary to analyze plant process dynamics and improve controls and equipment reliability.

4. RECOMMENDATIONS

Opportunities to promote and ultimately apply QIS to help achieve the goals of DOE-FE are provided in the previous sections. The near-term research opportunities that help explore the applications of QIS in fossil energy and help develop a workforce at the intersection of fossil energy and QIS are summarized in the following sections.

Sensors and Subsurface

Several quantum sensing modalities could become mature in the near term for fossil energy applications. Many of these sensors are for subsurface applications:

- Fiber optic sensors using squeezed light as the interrogating field could find applications in oil & gas extraction or carbon capture and storage. Measurements of interest include dynamic and static strain, magnetic fields, temperature, and others.
- Sensors relying on time order, or sensors relying on ultrafast optics or dynamics can benefit from entangled atomic clocks. In general, sensors benefitting from a universal frame for time and frequency measurements will perform with more accuracy if entangled clocks can be distributed over geographically relevant sites for oil & gas exploration. Furthermore, by invoking precision metrology afforded by entangled clocks, the frequency and amplitude of minute gravity oscillations associated with the breathing modes of earth may be detected. This can enable ultrafast and ultraprecise detection of the extent of explosion and gravity fluctuations, stress variation, presence of and displacement in fluids, etc., which can prove useful in better design and control in mining applications.
- Integrate diamond-based quantum sensing methods into microfluidic devices to provide new insights into the interfacial molecular structure and macroscopic properties of common and novel fluids for subsurface operations.
- Investigate the use of surface functionalized nano-diamonds such that they partition into foam lamellae to enable local molecular properties to be determined in situ and correlated with macroscale flow for subsurface operations.
- Use nitrogen-vacancy (NV^-) based dynamic nuclear polarization to hyperpolarize external nuclei. This method has the potential to dramatically reduce the time required to acquire physical and chemical data and introduce new applications, such as measuring flow rates in porous media.
- Investigate the use of atomic magnetometers to characterize porosity by detecting proton spin transitions in the Earth's magnetic field.
- Near-distance standoff photo-absorption techniques in the visible (vis) and near infrared (near-IR) spectral regions could be developed for detecting rare earth elements.

Power Plant, Electrical Grid, and Oil & Gas Cybersecurity

The most important near-term goal in the application of QIS to cybersecurity should be to make fossil energy devices "quantum ready," not only for quantum key distribution (QKD) but also for general quantum communication and networking that provides benefits beyond cybersecurity. Work on developing a flexible, extensible quantum-ready network architecture for fossil energy—one that can operate with quantum systems through common management and control— can start now. Such a system should demonstrate classical sensors protected by QKD as well as new quantum sensing mechanisms for all fossil energy industries.

Materials Development

Variational algorithms that utilize hybrid approaches, where both the quantum and classical computer are working in tandem, are proving to be useful to achieve effective quantum simulation. Such algorithms partly overcome current limitations in quantum computers. These computational approaches, known as hybrid quantum-classical algorithms, are suitable for currently available noisy intermediate-scale quantum (NISQ) computers. A near term opportunity is to conduct proof of concept quantum computing for the development of materials for fossil energy applications such as catalysts for direct methane conversion, oxygen carriers for chemical looping processes, sorbents and solvents for carbon capture, and materials for the storage of chemical, thermal, and electrical energy.

Powerplant Design and Optimization

A better understanding of both the potential benefits and challenges in the application of quantum computing to powerplant design and optimization is needed. Among the challenges is determining how to effectively map problems/data into quantum compatible forms and back to classical formulations to enable hybrid computing approaches. An exploratory research project among fossil energy optimization experts and quantum information scientists to develop effective mapping approaches for problems/data into quantum compatible forms and back to classical formulations would enable an interface between classical and quantum computing that could be used to rapidly demonstrate potential benefits of quantum computing on ongoing fossil energy systems optimization priorities.

Powerplant Operation and Control

Quantum optimization algorithms could potentially address several needs in power plant operation and control, such as real-time optimization of fuel/air ratio, optimizing the operation of control equipment for nitrogen and sulfur oxides (NOx and SOx), and improving the burner design. Quantum computing may also find applications in the compression of massive amounts of data generated by various process instruments and in using that high-fidelity data and enhanced understanding of real-time materials/chemistry and thermodynamics/heat transfer phenomena to make boiler component life predictions.

Other Areas

An area that needs attention is the development of performance benchmarks for quantum computing methods most relevant to fossil energy applications. This will help inform whether a quantum computer is better than a classical computer for a given application.

The development of workforce at the intersection of fossil energy and QIS need to be initiated. A step in that direction, for example, could be through NETL and Pittsburgh Quantum Institute collaborating on QIS research in sensing, computing, and networks applied to high priority fossil energy problems. Establishing other university projects and fellowship opportunities will help attract students to work at the intersection of fossil energy and QIS and gain expertise in QIS applications to fossil energy.

APPENDIX A. FOSSIL ENERGY WORKSHOP ON QUANTUM INFORMATION SCIENCE & TECHNOLOGY AGENDA

Find the entire Workshop Handout by *clicking here*.

TUESDAY, NOVEMBER 19, 2019

8:00 – 8:30 A.M.	**CHECK-IN/BREAKFAST**
8:30 – 9:00 A.M.	**WELCOME/INTRODUCTION** Randall W. Gentry (NETL) on behalf of Brian J. Anderson (NETL) Madhava (Syam) Syamlal (NETL) Jeremy Levy (U. of Pittsburgh/PQI)
9:00 – 9:30 A.M.	**DOE PROGRAM IN QUANTUM INFORMATION SCIENCE** Barbara Helland (U.S. Department of Energy)
9:30 – 10:00 A.M.	**KEYNOTE, FOSSIL ENERGY** Charles McConnell (U. of Houston)
10:00 – 10:15 A.M.	**BREAK**
10:15 – 10:45 A.M.	**KEYNOTE, QUANTUM INFORMATION SCIENCE** Celia Merzbacher (Quantum Economic Development Consortium)
10:45 – 12:15 P.M.	**PANEL 1 – QUANTUM SENSORS/DETECTORS AND QUANTUM EXPERIMENTS** Panel Moderator: Randall W. Gentry (NETL) Panel Members: Chethan Acharya (Southern Company), Henry Du (Stevens Institute of Technology), Carl Williams (NIST), Benjamin Lawrie (ORNL), Michael Hatridge (U. of Pittsburgh), Benjamin Gilbert (LBNL), Supratik Guha (ANL)
12:15 – 1:15 P.M.	**LUNCH**
1:15 – 2:45 P.M.	**PANEL 2 – QUANTUM COMPUTATION FOR MACHINE LEARNING, AI, AND OPTIMIZATION** Panel Moderator: David Miller (NETL) Panel Members: Zlatko Minev (IBM), Nick Sahinidis (Carnegie Mellon), Earl Scime (WVU), Aaron Hussey (Integral Analytics), John Siirola (SNL), Michael Flatté (U. of Iowa)
2:45 – 3:00 P.M.	**BREAK**
3:00 – 4:30 P.M.	**PANEL 3 – QUANTUM COMPUTATION/SIMULATION FOR CHEMISTRY AND MATERIALS** Panel Moderator: Jeremy Levy (U. of Pittsburgh/PQI) Panel Members: Philip Richerme (Indiana U.), Götz Veser (U. of Pittsburgh), Ignasi Palou-Rivera (RAPID Manufacturing Institute), Raphael Pooser (ORNL), Mike Santos (U. of Oklahoma), Andrew Baczewski (SNL)
4:30 P.M.	**ADJOURN**

WEDNESDAY, NOVEMBER 20, 2019

8:00 – 8:30 A.M.	**CHECK-IN/BREAKFAST**
8:30 – 10:00 A.M.	**PANEL 4 – QUANTUM COMPUTATION FOR PROCESS MODELING/CFD AND QUANTUM NETWORKING** Panel Moderator: Richard Bajura (WVU) Panel Members: Peyman Givi (U. of Pittsburgh), Michael Leuenberger (U. of Central Florida), Stephen Bush (GE), Randy Smith (SNL)
10:00 – 10:15 A.M.	**BREAK**
10:15 – 12:15 P.M.	**FACILITATED BRAINSTORMING SESSION – OPPORTUNITIES FOR FOSSIL ENERGY APPLICATIONS**
12:15 – 12:30 P.M.	**CLOSING REMARKS**
12:30 – 1:30 P.M.	**LUNCH**
1:30 P.M.	**ADJOURN**

APPENDIX B. LIST OF ACRONYMS

AAC	alternating current
AI	artificial intelligence
AIChE	American Institute of Chemical Engineers
ANL	Argonne National Laboratory
CFD	computational fluid dynamics
CLC	chemical looping combustion
CLBC	chemical looping beyond combustion
CURC	Carbon Utilization Research Council
DC	direct current
DNP	dynamic nuclear polarization
DOE	U.S. Department of Energy
DOE-FE	DOE Office of Fossil Energy
GPS	Global Positioning System
LBNL	Lawrence Berkley National Laboratory
LIGO	Laser Interferometer Gravitational-wave Observatory
ML	machine learning
MINLP	mixed integer nonlinear problems
MOF	metal organic framework
MRI	magnetic resonance imaging
NETL	National Energy Technology Laboratory
NIST	National Institute of Standards and Technology
NMR	nuclear magnetic resonance
NRCCE	National Research Center for Coal and Energy
NREL	National Renewable Energy Laboratory
NSF	National Science Foundation
NV	nitrogen vacancy
ORISE	Oak Ridge Institute for Science and Education
ORNL	Oak Ridge National Laboratory
PQI	Pittsburgh Quantum Institute
QKD	quantum key distribution
QNR	quantum noise reduction
QRNG	quantum random number generation
REE	rare earth element
SNL	Shot Noise Limit
SNL	Sandia National Laboratories
SNR	signal-to-noise ratio
sCO2	supercritical carbon dioxide
TPM	Trusted Platform Module
WVU	West Virginia University
WQC	wireless quantum communication
WQKD	wireless quantum key development

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QUANTUM INFORMATION SCIENCE & TECHNOLOGY

SUMMARY REPORT

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