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Exploring the potential landscape of chemical engineering science

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As part of the first anniversary issue of *Nature Chemical Engineering*, we present a collection of opinions from 40 researchers within the field on what they think are the most exciting opportunities that lie ahead for their respective topics.

Modern chemical engineering is undergoing a marked phase transition. The field has built and dramatically expanded upon its roots in industrial process engineering over the past several decades; the pace of this transformation continues to grow in response to both scientific advances and time-sensitive societal and environmental challenges. This critical point provides an opportune moment to consider where the field and practice of chemical engineering may be heading, and what new science may again transform the field over the coming years. In this Feature, we sample this potential scientific landscape by asking 40 members of the community to share their perspectives on the most exciting opportunities that lie ahead for their respective topics. While our sample size is finite, this collective viewpoint captures a broad and diverse snapshot of the contemporary driving forces in chemical engineering practice. Here is what they said.

Claire S. Adjiman

To meet the world's needs for sustainable chemicals, we must move beyond the idea of inherently 'green' molecules to a more holistic approach that encompasses the entire chain of production and consumption, including atoms, devices, processes and products. This means creating a new molecular systems engineering approach to design molecules and materials based not on their properties but on the performance of the whole supply chain. By building on rapid progress in computational chemistry, high-throughput/automated experimentation, multi-scale modeling and optimization, we have a unique opportunity to create the decision-making tools that will transform the way in which engineers design industrial systems.

Panagiota Angeli

Intensified separations in small channels have emerged as a transformative solution for the transition to sustainable solvent extractions and can aid the industrial uptake of non-petroleum-based solvents. Flow separations in small channels integrated with sensors and coupled with predictive models will enable dynamic and adaptive process operations. These will form the basis for digital twins for separations, which flexibly respond to varied and changing feed streams, without compromising the quality and specifications of the final product. Such technologies will be able to handle challenging separations such as those involved in the recovery of metals from electronic waste, spent magnets or batteries, thus addressing environmental issues and supporting circular economies.

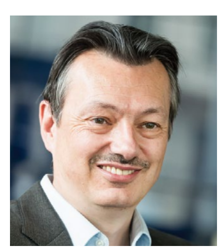
André Bardow

Climate change and chemical pollution force the chemical industry to ask itself: "If we could do it all over again, how would we do it better?" This dilemma requires us to rethink our industry from cradle to grave: switching to renewable feedstocks and energy in intensified processes, implementing a circular economy while providing safe and sustainable products for an ever-growing population. Developing each of these elements leads to formidable research questions. A key challenge is ensuring these elements will ultimately fit together. While this task might seem daunting, I am optimistic that chemical engineering thinking can enable a sustainable chemical industry.

Stacey F. Bent

Chemical engineers will be critical in helping achieve advances in materials processing that are required for next-generation microelectronics. Explosive global trends in artificial intelligence, machine learning, Internet of Things, autonomous transportation and more are driving huge needs for ever-faster, cheaper and more energy-efficient chips for both logic and memory. Existing microelectronics devices are already marvels of decades of engineering achievement, but new frontiers demand continual improvement. Developing the chemical control to manipulate the placement and quality of component materials at the nanometer scale and in complex three-dimensional device structures is a huge and exciting challenge in the field.

Nigel Brandon



Fuel cells will play a key role in the low-carbon transition, offering highly efficient, clean and flexible conversion of a wide range of green fuels (such as hydrogen, ammonia, methanol and ethanol) into power, be this for transport applications such as trucks,

CREDITS: ETH ZÜRICH, JAKOB INEICHEN (MIDDLE); ALEX GILLASPY, STANFORD UNIVERSITY (TOP RIGHT) trains, ships and aircraft, or for power generation for data centers or grid reinforcement. Key areas of opportunity for innovation are in new electrocatalysts, new high-temperature ion-conducting membranes and reduced use of rare or critical materials. In addition, scaling up fuel cell technology through stack and system engineering, supported by low-cost volume manufacturing, is essential.

Katie Galloway

Solving the problem of scalable production remains one of the greatest challenges in delivering on the promise of gene and cell therapies. To produce therapeutic vectors and for them to serve as cell-based therapies requires better models for understanding cells as systems and improved tools for engineering precise control around cellular processes. Through mathematical modeling and use of fundamental principles in kinetics, thermodynamics and transport, chemical engineers are uniquely positioned to enhance our understanding and to design systems — across molecular- to production-level scales — that can solve the challenge of scalable production.

Raymond J. Gorte

Ideally, heterogeneous metal catalysts would exhibit high-temperature stability and the high selectivity of homogeneous catalysts. New synthesis methods, especially atomic layer deposition, allow preparation of thin oxide films on stable supports with unprecedented control of composition and structure. Some thin-film mixed oxides with a perovskite structure can dramatically suppress sintering of supported metal particles. Other mixed oxides can act as supports for single metal atoms, stabilizing them and acting as ligands to promote catalytic properties, analogous to ligands in homogeneous complexes. These thin-film materials and their interactions with supported metals should provide for better control over catalyst activity and selectivity.

Gonzalo Guillén-Gosálbez

Sustainable process systems engineering will be key for guiding technology development and deployment toward sustainability. We will witness substantial growth in life-cycle optimization applications within chemical engineering (for example, electrification of operations and shift to renewable carbon) and beyond. How to cover data gaps in life-cycle assessment (LCA) and quantify the broad implications of engineering decisions will attract much attention. The latter will require building and solving multi-scale and cross-sectoral multi-objective models under uncertainty including LCA-based absolute sustainability metrics. Incorporating sustainability topics in the curriculum and interacting closely with policymakers will be crucial to further catalyze the sustainable transition.

Claudia Gutiérrez-Antonio

Sustainable aviation fuels are key to decarbonizing the aviation sector. Sustainable aviation fuels can be produced from a wide range of biomass feedstocks through different conversion pathways that can meet technical American Society for Testing and Materials (ASTM) standards. Moreover, such biofuels can reduce up to 80% of greenhouse gas emissions in their life-cycle. One key challenge relies on reaching economic competitiveness. For this, the conversion of complete biomasses, virgin or residuals, through a biorefinery is promissory, since profitability relies on several products. Therefore, sustainable aviation fuel biorefineries are an ideal flight plan to move from the laboratory to the sky.

Marta C. Hatzell

There has been a significant push over the past decade to develop more sustainable chemical manufacturing processes to make agrochemicals. This is largely driven by the global need to meet net-zero carbon emissions within the chemical sector. I am excited for the next decade of research in this field, as I believe many of these new electrified chemical manufacturing processes based around electrochemical, photochemical, plasma-based reactors will move toward piloting and commercialization. The real challenge with these new chemical manufacturing processes will be driving down cost and ensuring that environmental impacts are adequately addressed from a systems-level perspective.

Michael C. Jewett

Cell-free systems empower synthetic biologists to build biological molecules and processes outside of living, intact cells. This concept advances fundamental understanding of how nature works the way it does, circumvents mechanisms that have evolved to facilitate species survival and makes possible an entirely new vision of distributed biotechnologies. Maturing areas of innovation include cell-free synthesis of new-to-nature molecules and materials, machine-learning-guided cell-free platforms that link protein design and protein function, and scale-up of protein and biomolecule production. Use-inspired applications will transform health, manufacturing, sustainability and education.

Marlene Kanga AO

Chemical engineers have a crucial role in developing innovative solutions to enable the transition to lower-emissions technologies and tackle the imperative to address climate change and a net-zero future. Chemical engineers also need to develop tools and strategies to address any new systematic safety risks that may arise with the development of new processes. The Institution of Chemical Engineers (IChemE) Safety Centre with 120 member organizations globally is developing strategies and programmes to build capacity for systematic approaches to process safety, developed for hazardous industries over the past 50 years, and applying these to other sectors. This is essential for a just transition and for our sustainable future.

Michael Köpke

Biological engineering and biomanufacturing have immense potential to tackle our grand challenges and revolutionize our economy. After 50 years of research, we are at an exciting inflection point with the emergence of modern gene editing and protein design techniques. Advancements in artificial intelligence (AI) will further transform the future of the field, but biological systems are complex. To fully harness the power of AI, large-scale biological datasets across multiple systems and scales are needed, where modern biofoundries will play a key role. Biomanufactured products are already part of our daily lives, but further bioprocess scale-up advancements will be critical to foster competitiveness, including utilization of waste-based feedstocks and continuous processing.

Markus Kraft

Digitalization and artificial intelligence (AI) are already having a profound impact on chemical engineering in academia and industry. However, two problems still persist: lack of interoperability and hallucination of generative AI. I argue that explicit knowledge representation will overcome hallucination through reasoning and allow interoperability. The semantic web stack and in particular knowledge graphs may offer solutions as they allow the representation of data but also concepts associated with these data. While there have been successful case studies for material discovery, laboratory automation, plant control and smart energy grids, the technology is still in its infancy. Given the potential benefits I expect a rapid expansion of this field.

Ung Lee

One exciting aspect of chemical engineering research is the advancement of CO_2 reduction technologies, offering a sustainable way of mass production for commodity chemicals. This alternative approach will lead to new developments in many aspects of chemical engineering, such as catalyst design, reaction engineering and process systems engineering. Critical requirements for CO_2 utilization technology are providing a large amount of renewable energy for the CO_2 conversion process and developing means to integrate the dynamic supply of energy into the production system. Addressing these challenges is essential for driving innovation and ensuring the sustainability of future industrial practices.

Yayuan Liu

There is a pressing need to develop more sustainable, non-thermal separation processes that can address urgent challenges such as carbon emissions and resource scarcity. Achieving this requires the innovative integration of diverse approaches, including precise molecular and materials design, electro- and photochemistry, interfacial science, transport and non-equilibrium phenomena, advanced characterizations, and data science tools, among others. Equally crucial is the application of core chemical engineering principles — such as multi-scale modeling, device engineering, process intensification and system-level assessments — to expedite the translation of these novel separation solutions into real-world applications, thereby accelerating our transition to clean energy and a circular economy.

Guanghui Ma

An exciting challenge in vaccine engineering lies in applying biochemical engineering principles to quantify and interpret the complex biological processes that occur in vivo. For instance, vaccine delivery that overcomes in vivo barriers, as well as immune responses dependent on cellular interactions, exemplifies the concepts in bioprocess engineering. However, the intricate interplay between delivery kinetics and the subsequent immune response remains largely a 'black box'. Drawing on our 20 years of high-quality experimental data, machine learning and computational simulation offer promising tools for the rational design of effective and safe vaccine delivery systems, potentially accelerating the vaccine development process.

Ewa Marek

We are witnessing enormous progress in materials discovery, but a large gap exists in translating those discoveries into implementable and scalable applications. Bridging this gap is not trivial and requires a comprehensive way of linking information between disciplines to finally reach a holistic understanding of property–stability–performance relationships. While much research is already dedicated to building this understanding, the efforts need consolidating and translating into one 'common language'. Another exciting avenue, also in my work, is the development of inherently transient and cycling processes, such as chemical looping, plasma-supported reactions, or sono- and mechanochemistry, which will help reshape the chemical industry into an agile, renewably powered sector.

Massimo Morbidelli

Biopharmaceuticals provide a substantial fraction of the therapeutic tools available today for medical care. Monoclonal antibodies have been shown effective for cases such as cancer and autoimmune diseases. Gene and cell therapies are being established as a new paradigm in medical care. Such extraordinary innovations open opportunities for treating an increasing number of patients but require more efficient bioprocesses for their production. Digitalization and automation, in connection with continuous and fully integrated manufacturing, will help to provide biopharmaceuticals to all patients who need them. This means revolutionizing how we make biopharmaceuticals, and provides a tremendous opportunity for the next generation of chemical engineers.

Eranda Nikolla

Heterogeneous catalysts are essential to a sustainable and future renewable energy platform that addresses contemporary challenges associated with fossil fuel energy and environmental pollution. Exciting directions in catalyst design include engineering the local environment around the active site, identifying ways to overcome scaling relations and understanding their dynamic nature under reaction conditions. Advancements in these areas hinge on new synthesis approaches, in situ and operando techniques, and computational tools to effectively correlate catalyst surface structure with catalytic function. Critical to the success of catalyst design is the effective evaluation of their function, which requires implementation of benchmark protocols to ensure rigor and reproducibility across the field.

Maria Papathanasiou

We are navigating an era when machine learning and artificial intelligence are at the center of computer modeling attention. Understanding how to purposefully use such tools and maximize their potential by combining them with traditional, physics-based approaches is key. The development of holistic frameworks for the construction of hybrid models is now time critical and will pave the way toward next-generation computer modeling tools that can interact with data and humans in an ethical and efficient manner.

Ah-Hyung Alissa Park

Creating a circular carbon economy with net-zero emissions is one of the biggest challenges faced by humanity. One of the exciting frontiers in carbon capture and conversion research is the electrification of chemical reactions and separations utilizing renewable electrons to convert CO_2 to useful products. We are now just beginning to understand how non-thermal energy transfer mechanisms can be employed to heat, activate and transform CO_2 in scalable ways. I believe this new research direction requires innovative in situ and operando measurements at interfaces, as well as artificial-intelligence- and machine-learning-driven studies to investigate coupled reaction and transport behaviors across many scales.

Ingo Pinnau

Polymeric-membrane-based separation processes have reduced the energy cost and environmental impact of conventional thermally driven unit operations. Designs of carbon molecular sieves, polymers of intrinsic microporosity, metal–organic frameworks, two-dimensional materials and others have generated ultra-selective and high-productivity membrane materials. These emerging materials can potentially be applied to replace or de-bottleneck conventional processes for hydrogen purification, olefin/paraffin splitting, CO_2 capture, micropollutant removal and ion/ion separation for brine mining. However, the lack of innovative low-cost techniques to process new bulk materials into high-performance thin-film membranes has severely limited further expansion of membrane technology and needs to be addressed in future research.

Shi-Zhang Qiao

Thanks to the development of nanotechnology, a variety of high-performance electrocatalysts have been synthesized in laboratories, with applications in fuel cells, water electrolyzers and batteries. However, disparities exist between fundamental research and practical device demands due to differences in gas and liquid transport, reaction environments, system design and fabrication. To bridge these gaps and industrialize advanced nanomaterials for practical clean energy devices and applications, an exciting frontier lies in electrochemical engineering. This interdisciplinary approach integrates the principles of chemical engineering, materials science, electrochemistry and mechanical engineering to drive sustainable energy solutions.

Vivek V. Ranade

Reducing side products and emissions from multi-phase reactors is essential for sustainable chemical production. This requires ensuring the delivery of materials and energy at the right time and place within these reactors. A key barrier is the lack of high-accuracy models anchored to real-world reactors. Wall pressure fluctuation data acquired from industrial reactors capture critical information about multi-scale transport processes and offer a promising solution for anchoring models to reactors without arbitrary adjustable parameters. Further research into combining physics-based models with these data via machine learning presents exciting opportunities to develop accurate reactor models. Such models can drive strategic interventions and targeted improvements, paving the way for more efficient and sustainable processes.

Luis Ricardez-Sandoval

Machine learning algorithms as well as advanced optimization methods can aid in the design, operations management and intensification of complex chemical and manufacturing systems. They can also accelerate the discovery of new systems and materials to enhance the sustainability of emerging and existing processes. Recent contributions have shown the potential of such methods to accomplish challenging tasks in chemical engineering, for example, automatic generation of process flowsheets using reinforcement learning. Going forward, efficient computational and communication frameworks must be developed to consider detailed modeling aspects taking place at multiple temporal and spatial scales. This enables the ultimate goal of designing intensified and sustainable materials and systems involving atomistic, molecular and macroscopic scales.

Sindia M. Rivera-Jiménez

The chemical engineering curriculum must embrace the exciting challenge of integrating lifelong learning and social impact. I envision a transformative model where education researchers, faculty and industry partners collaborate to create contextualized learning environments that connect content to students' real-world experiences and interests. These environments will prepare students to tackle critical challenges such as sustainable energy, advanced manufacturing, healthcare innovation and environmental stewardship. By prioritizing inclusivity and valuing diverse perspectives, departments can bridge academia with industry, nurturing talent to drive meaningful societal change and thrive in a technology-driven future.

Kirti Chandra Sahu

A major challenge in predicting weather accurately lies in the limited understanding of the microphysical processes that govern atmospheric phenomena. Empirical relationships commonly used in weather radars for rainfall estimation rely on parameters such as raindrop size distribution at different altitudes, which involve assumptions and uncertainties. These parameters are influenced by intricate microphysical processes, such as droplet fragmentation, coalescence and phase change, which are further affected by region-specific factors such as temperature and humidity. Current weather models tend to oversimplify these complexities, compromising their predictive accuracy. Chemical engineers are uniquely positioned to bridge this gap by developing advanced models and conducting precise experiments to enhance weather forecasts.

Berend Smit

The potential of metal–organic frameworks lies in their customizability for specific applications. If one can make a nearly infinite number of materials, finding the optimal one for, say, carbon capture processes requires novel methodologies in which artificial intelligence (AI) will play a crucial role. However, even the best AI methodology will not have any impact if its objective function is not identified properly. The scale of any climate mitigation strategy requires a holistic approach that integrates AI with the fundamentals of chemical engineering, that is, materials properties, process design, techno-economics and life-cycle assessment, to identify such an objective function.

Randall Q. Snurr

An exciting recent development in chemical engineering — and science and engineering more broadly — has been the increasing availability of open-source software. While the Internet clearly opened up possibilities for communication that did not exist a generation ago, there has also been a healthy shift in mindset where sharing software is now acknowledged and valued. Instead of spending weeks writing code from scratch, today's researchers can often find helpful tools online. The availability of code ranging from large simulation packages to customized scripts makes research more reproducible, saves tremendous amounts of researcher time and is greatly accelerating the pace of research and development.

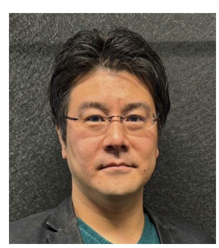
Cíntia Soares

Computational chemical engineering will expand significantly in the coming decades, driving advancements in the chemical industry. One major challenge is accelerating the solution of accurate multiscale, multi-phase and multi-physics models that capture essential phenomena in intensified equipment, such as photochemical and electrochemical reactors. Overcoming this is crucial for effective design, optimization and scale-up strategies. A promising strategy involves integrating computational fluid dynamics with reduced-order models for high-performance predictions. Additionally, the shift toward graphics processing unit (GPU)-based computational fluid dynamics codes is expected to be transformative, enabling faster and more efficient simulations, revolutionizing complex system analysis and fostering sustainable innovation in process engineering.

Kevin Solomon

Microbial biomanufacturing promises sustainable routes to the chemicals that drive modern society, and more importantly, may deconstruct them at end of life. A grand challenge of the field is developing microbial platforms that use abundant waste materials including plastics such as polyethylene. Natural systems hint at the feasibility of such systems; however, we currently know little about the enzymes that facilitate this under ambient conditions. Powerful techniques in systems biology and chemical biology promise to identify these enzymes, which may be optimized with emerging techniques in engineering biology and machine learning to create truly scalable solutions for a circular economy.

Kazuhiro Takanabe



Green hydrogen production by water electrolysis is an urgent issue. The more I experiment with water electrolysis, the more I am captivated by the mystery of water. We have not yet been able to fully describe the electronic structure and physical properties of water. Basic properties such as solubility of substances and ions, conductivity, viscosity, diffusion coefficient, Pourbaix diagram of quasi-stable phases and reactivity of water at interfaces have not yet been theoretically quantified fully. It is gratifying to see new chemistry of electrocatalysts emerging through 'electrolyte engineering' to maximize electrolytic performance, which is being pursued concurrently with 'electrode engineering'.

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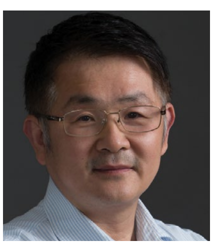
Xiaonan Wang

As an inherently interdisciplinary field, chemical engineering is naturally aligned with computer science and artificial intelligence (AI), especially with numerical methods and data science. We have been developing active learning strategies and foundation models to not only accelerate the development of chemicals and processes, but also to provide insights that could lead to breakthroughs in materials, systems and theoretical hypotheses. Crucially, AI-driven approaches in catalyst design and catalytic process optimization are substantially enhancing discovery efficiency and supporting sustainable development toward a net-zero future. The synergy between computer science and chemical engineering embraces a future of exciting advancements, driving innovation and sustainability in the field.

Fei Wei



Fossil energy has been a cornerstone for economic vitality; however, its use in conventional chemical engineering processes is marred by significant CO_2 emissions, an unresolved environmental challenge. Looking ahead, the forthcoming decade should prioritize the development of advanced catalysts that facilitate the transformation of CO_2 into sustainable fuels or high-value chemicals. In the realm of transportation, particularly for heavy-duty vehicles, the transition to electrification is not yet feasible, given their reliance on liquid fuels. Consequently, there is an urgent need to innovate toward cleaner synthetic fuel alternatives that substantially reduce the environmental footprint by minimizing pollutant emissions.

Matthias Wessling

The natural world exemplifies the seamless integration of chemical and redox reactions with molecular separations, driving the complex processes that sustain life. Inspired by nature's design principles, the next frontier in synthetic membranes lies in harnessing this synergy to create integrated material systems such as electrochemical membrane reactors. By integrating chemical and redox functionalities with synthetic membranes, unprecedented control over molecular interactions and separations will be unlocked. This integrative and nature-inspired approach will pave the way for transformative advancements in energy, biotechnology and environmental solutions, contributing viable solutions to the most pressing global challenges of our time.

Kathryn Whitehead

Although there are RNA vaccines and treatments for liver disease, an outstanding challenge is delivery to other organ and cell targets. One exciting avenue is addressing this challenge using chemically complex and highly modular nanoparticles that, with small changes in chemistry, transport RNA to new organs such as the brain and pancreas. As chemical engineers, we are in love with the exquisite effects of nanoparticle chemistry on delivery efficacy and toxicity. We and others are now uncovering the chemical mechanisms that control delivery and are expanding the nanoparticle formulation space, which we hope will enable treatment of any human disease, no matter its location.

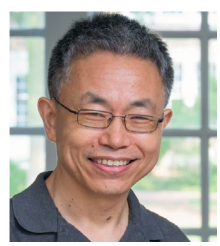
John M. Woodley

Thanks to developments in metabolic engineering and protein engineering, today many new bioprocesses are being developed in the laboratory. Some bioprocesses make novel products (in particular, proteins), which cannot be made in any other way. Others make (chemical) products from alternative starting materials. The latter often make use of enzymatic biocatalysts resulting in high-productivity processes, but placing special demands on scale-up. A very exciting area of chemical engineering today is the creation of scale-down mimics reflecting new-to-nature industrial conditions and gradients. Using such apparatus, biocatalysts can be investigated under new conditions and models developed for effective scale-up.

Zaiku Xie

Catalytic technology, the cornerstone of the modern chemical industry, facilitates the conversion of diverse chemicals. High atom economy and greener manufacturing processes are urgently desired in catalysis. The challenges lie in the precise design and synthesis of catalysts, control of reaction and diffusion pathways, and optimization of reaction engineering. It is thus essential to address some critical fundamental issues such as reconstruction of active sites, dynamic evolution of intermediates, and diffusion kinetics at the microscale by combining advanced in situ/operando characterization techniques and computational approaches. A sustainable future can be envisaged with the substantial development of catalysis science and technology.

Yushan Yan



Electrochemical engineering is a branch of chemical engineering that focuses on the design, scale-up, optimization and economics of electrochemical processes. Pioneered by Charles Tobias at Berkeley in the 1950s, modern electrochemical engineering has been experiencing a renaissance as the world moves toward a net-zero future. To adequately decarbonize our economy, electrochemical devices such as electrolyzers, fuel cells and batteries have begun to play a central role, and electrochemical engineering has become a new frontier of chemical engineering innovation. The key to the success of electrochemical devices is cheap and abundant green electricity, inexpensive and durable materials and simpler reactor design for fast, massive-scale manufacturing.

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Competing interests

The authors declare no competing interests.