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Artificial Intelligence and Machine Learning for Sustainable Molecular-to-Systems Engineering

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ABSTRACT

Sustainability encompasses many *wicked problems* involving complex interdependencies across social, natural, and engineered systems. We argue holistic multiscale modeling and decision-support frameworks are needed to address multifaceted interdisciplinary aspects of these wicked problems. This review highlights three emerging research areas for artificial intelligence (AI) and machine learning (ML) in molecular-to-systems engineering for sustainability: (1) molecular discovery and materials design, (2) automation and self-driving laboratories, (3) process and systems-of-systems optimization. Recent advances in AI and ML are highlighted in four contemporary application areas in chemical engineering design: (1) equitable energy systems, (2) decarbonizing the power sector, (3) circular economies for critical materials, and (4) next-generation heating and cooling. These examples illustrate how AI and ML enable more sophisticated interdisciplinary multiscale models, faster optimization algorithms, more accurate uncertainty quantification, smarter and faster data collection, and incorporation of diverse stakeholders into decision-making processes, improving the robustness of engineering and policy designs while focusing on the multifaceted goals and constraints in wicked problems.

Keywords: Artificial Intelligence, Machine Learning, Multiscale Modelling, Interdisciplinary, Optimization

INTRODUCTION

Creating engineered solutions to help achieve UN sustainable development goals (e.g., clean water and sanitation, affordable and clean energy, responsible consumption and production), [1] requires managing complex trade-offs across diverse molecular, material, device, process, and infrastructure scales[2]. As such, breakthroughs at a single scale are often insufficient to realize global impact. Moreover, these *wicked problems*[3,4] require interdisciplinary teams to manage interdependencies across social, natural, and engineered complex systems.

Using four contemporary sustainability challenges in chemical engineering, this short paper argues recent advances in artificial intelligence (AI) and machine learning (ML) methods for product and process design offer new capabilities to accelerate decision-making across molecular-to-system length and timescale. For brevity, we direct the reader to several excellent review articles and editorials for technical overviews of AI[5,6], ML[7–11], and data science (DS)[12–14] methods used in chemical engineering. This paper focuses on advances and opportunities for AI, ML, and DS for product and materials design, which we argue is inherently multiscale and interdisciplinary. Many now consider AI as an academic discipline, and ML is a field within AI[15]. Similarly, DS is an interdisciplinary field focused on extracting knowledge from data, which historical roots in applied statistics[16]. We do not dwell on the formal distinction between AI, ML, and DS.

MOTIVATING APPLICATIONS

We start by framing four sustainability challenges, each of which presents many opportunities for innovations in designing materials, products, and processes. However, fully realizing the benefits of technology development requires holistic systems engineering approaches, which AI and ML help facilitate.

Equitable Energy Transitions

Social, natural, and engineered systems around the

globe must adapt to climate change[17]. While the poorest and most marginalized have contributed minimally to global emissions, they are impacted the most by climate change[18]. Thus, it is critical to consider equity and environmental justice dimensions of technologies and policies to transition the global energy economy from fossil to renewable resources. Decision-making must consider many objectives and perspectives from diverse stakeholders[19] to manage complex interdependencies across social, natural, and engineered systems. Best practices to broaden representation in policy processes[18] can be integrated with systems thinking to enable participatory research on materials and chemical products focused on the authentic needs of poor and marginalized communities.

Decarbonizing the Power Sector

A key aspect of climate adaptation is decarbonizing electricity generation through greater adoption of carbon-neutral or renewable energy sources. One key technical challenge is that non-dispatchable renewable sources, carbon capture systems, and nuclear generators are often less flexible than fossil fuel generators. New sources of dynamic flexibility are needed to continuously balance electricity generation and production and ensure resiliency to extreme events (e.g., weather). Technoeconomic analysis of grid-connect systems, including power generators, storage systems, building, and (chemical) manufacturing processes, must consider the time-varying value of electrical energy, ancillary services, and demand response incentives[20–23] while considering uncertainty[24] and trade-offs between flexible operation and emissions[25]. Moreover, systems modeling can help inform the value of flexibility[26,27] and set performance targets for materials development, e.g., degradation in energy storage systems[28]. However, introducing new generators, energy storage, or integrated energy systems can distort prices in energy markets[29,30], which emphasizes the need for system-of-systems modeling to assess the economics of new technologies properly. Expansion planning[31,32] and similar decision-support tools[33] are needed to establish multi-decade decarbonization pathways[34,35] that ultimately inform materials design and technology development.

Circular Economies for Critical Materials

Reducing society's carbon footprint requires robust supply chains of critical minerals and materials (CMMs), including rare-earth elements (REEs)[36]. CMMs and REEs are essential to modern technologies, including energy storage, permanent magnetics in high-efficiency motors, and wind turbines. However, primary sources of REEs (and many CMMs) are environmentally costly to extract, separate, and refine[37]. Moreover, global pandemics, policies, and geopolitics can complicate CMM and REE supply chains[38,39]. Thus, there is a need for new materials that enable new separations and processes to recycle CMMs and REEs from distributed sources such as used batteries and consumer electronics[40]. In these proceedings, Dougher et al.[41] elaborates on opportunities for process systems engineering to accelerate membrane separations for CMMs and REEs.

Next Generation Heating and Cooling

As part of climate adaptation, recent international agreements mandate the phaseout of hydrofluorocarbon (HFC) refrigerants due to their high global warming potential. However, recycling existing HFCs requires new materials such as membranes[42,43], sorbents[44], ionic liquids[45–51], and deep eutectic solvents[52] to separate (near)-azeotropic mixtures. Beyond vapor recompression systems, new technologies such as solid-state devices may improve performance and lower carbon footprints[53]. Similarly, thermoelectric materials and devices can be engineered to power distributed electronics or convert waste heat into electrical energy[54]. These technologies require sophisticated co-optimization of materials composition[55], manufacturing processes[56,57], and device designs while considering performance targets from systems models.

Policy-mandated phase-outs and transformations in the heating and cooling section provide another example of complex interactions between social, natural, and engineered systems[58]. Systems-of-system models are needed to understand the development of HFC recycling supply chains and consumer behavior, e.g., adopting new technologies to establish a circular economy, especially considering changing climates. For example, policy interventions may be needed to ensure that next-generation heating and cooling technologies remain affordable for everyone. New materials and technologies must be benchmarked using systems models that capture these complexities.

AI & ML FOR MOLECULAR-TO-SYSTEMS

These four motivating examples emphasize the complexities of engineering new materials, chemical products, and processes to help meet sustainable development goals. This section highlights recent advances in AI and ML to address these challenges.

Molecular Discovery and Materials Design

Computer-aided molecular design (CAMD) methods integrate predictive models to engineer novel molecules and materials, often in conjunction with processes[59,60]. Classic examples include co-optimizing refrigerants and refrigeration cycles, creating *designer solvents* (e.g., ionic liquids) for a wide range of separations and reactions (e.g., CO_2 capture, crystallization, pharmaceutical manufacturing), and engineering new materials for

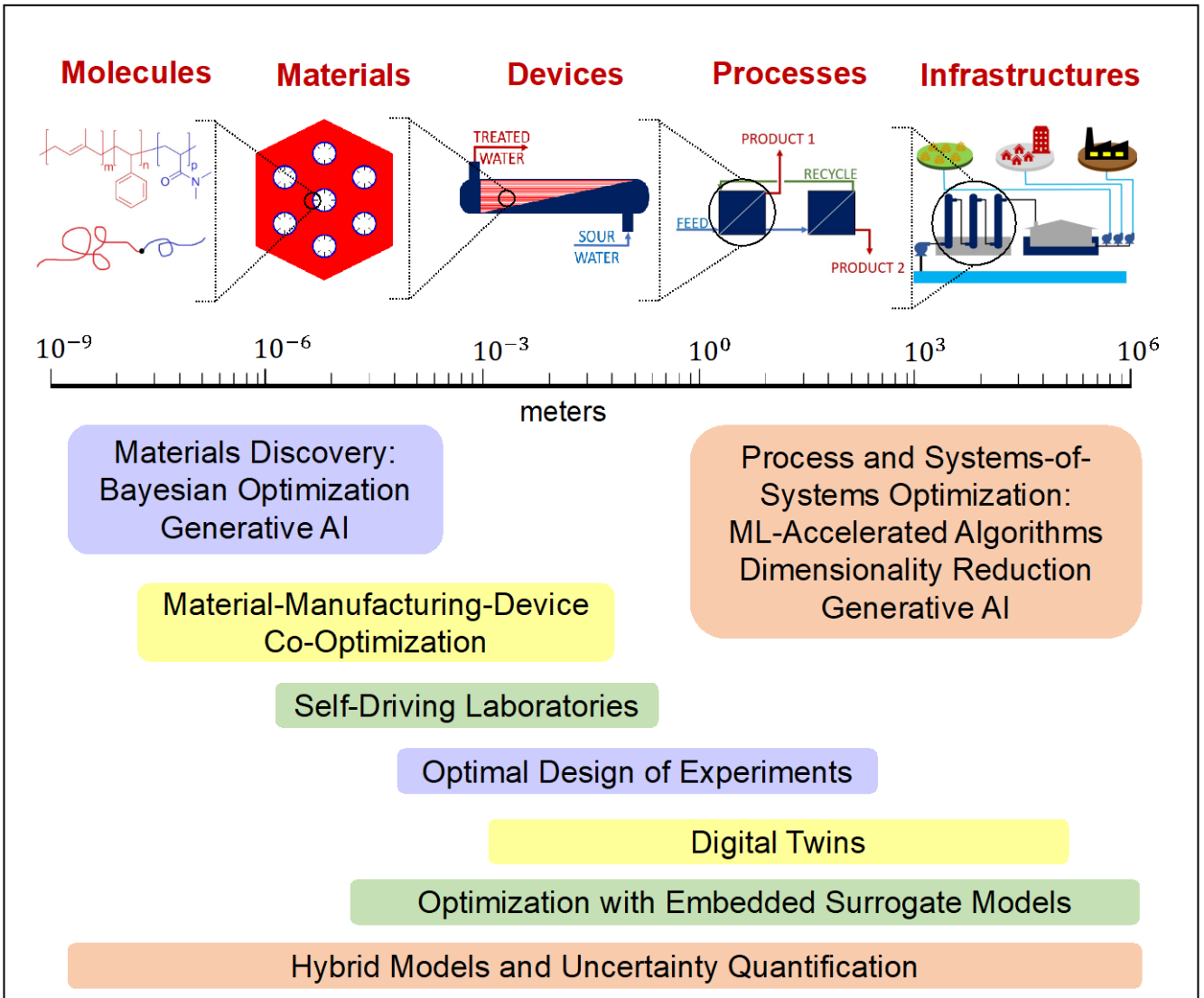

Figure 1: Overview of opportunities for AI and ML to accelerate molecular-to-systems engineering (adapted from

energy storage (e.g., electrolytes). Advances in deep learning[61] combined with massive datasets enabled by new data/text mining[62] can provide CAMD approaches with more accurate models to predict thermophysical and mixture properties as a function of molecular/materials structure.

Molecular simulations accelerate the engineering of new molecules and materials by providing new scientific insights or predicting properties at conditions impractical to measure. AI and ML offer several opportunities to improve the speed and accuracy of molecular simulations[63]. For example, ML surrogate models and Bayesian Optimization (BO)[64] can improve the speed and accuracy of parameter estimation for force fields[65,66]. We proposed[67] and refined[68] an ML-assisted optimization workflow to develop new force fields for seven refrigerants. Moreover, these physically interpretable force fields accurately predict properties not considered in calibration[69]. An alternative approach is to replace the force field expression with an ML model[70,71]. Both ML approaches are important because the lack of accurate force fields has historically hindered the use of molecular simulations to engineer some new classes of chemical products and functional materials.

Generative AI methods are emerging to engineer new molecules, materials, and synthesis pathways[72,73]. One popular approach uses variational autoencoders to reduce molecular descriptors into a latent space. BO[64] or reinforcement learning[74] can then optimize molecules in the latent space. ML frameworks are also emerging to co-optimize the material design, manufacturing, and end-use. For thermoelectric materials, we recently developed data science and BO methods to optimize photonic sintering[57] (advanced manufacturing), aerosol jet printing[56] (additive manufacturing), and dopant composition[55] (material design). These studies combined ML with expert intuition and laboratory experiments.

Automation and Self-Driving Laboratories

Self-driving laboratories (SDLs) are revolutionizing molecular discovery and materials design by combining recent advances in robotic automation with ML[75,76]. Most SDLs use black-box data-driven ML models to predict experiment outcomes (e.g., material properties, synthesis yields) from input decisions. AI methods such as BO or active learning plan the next sequence or batch of experiments. SDLs have successfully optimized materials and chemical syntheses, including learning the Pareto trade-offs between competing objectives, e.g., material properties[77].

Many functional materials for unit operations need to be optimized in the context of broader systems, which is likely too complex for SDLs with only data-driven ML models. For example, designing new membranes is not as simple as maximizing one property, such as selectivity or permeability, but instead, deciding how to balance material properties in the context of the broader separation system[78,79]. Instead, we propose combining automation and dynamic experiments for membrane characterization with science-based mathematical models[80]. Then model-based design of experiments methods[81] can be used to first distinguish between competing transport mechanisms and then optimize experiments to reduce model uncertainty. ML surrogate models can help reduce the computational burden of optimal experiment design[82] and model calibration[83]. Ultimately, this approach results in mathematical models with quantified uncertainty, i.e., digital twins[84], for process and infrastructure scale optimization.

Process and System-of-Systems Optimization

AI and ML provide new capabilities to improve the computational tractability, accuracy, and ease of implementation of integrated multiscale optimization across molecular, material, device, process, and infrastructure scales.

ML hybrid[83,85] or reduced-order surrogate models provide new scale-bridging approaches, especially considering the recent advances in computational optimization with embedded ML models[86,87]. For example, Rall et al.[88] used artificial neural network (ANN) surrogate models to incorporate high-fidelity ion transport membrane model performance predictions into the global superstructure optimization of a separation process. This methodology is especially powerful because it integrates rigorous models from another discipline (e.g., membrane science) with process systems engineering analyses. There is a significant opportunity for surrogate models to quantitatively establish (membrane) material property and device performance targets using process and systems models[78,79].

Similarly, ML surrogate models can enhance systems-of-systems modeling. For example, Jalving et al.[89] trained ANN surrogate models to predict how replacing/retrofitting a generator impacts transmission network-wide outcomes in a wholesale electricity market. These ANNs were then embedded into the steady-state co-optimization of generator design and operation. This example highlights the complex interactions between individual agents (e.g., generators) in the context of a larger system (electric market). In the broader sustainability context, systems-of-systems models combine economic, societal, and environmental submodels[90,91]. ML surrogate models provide new opportunities to further integrate these with technology submodels (e.g., materials, processes, supply chains, infrastructure) while leveraging multi-objective computation optimization. Moreover, ML surrogate models can enable next-generation decision-support tools where diverse stakeholders interact in real time with system-of-system optimization models to facilitate negotiations. Data reduction and visualization approaches are critical to understanding and explaining trade-offs between tens or more (often correlated) objectives in sustainability problems[25].

ML also provides new methods to quantify and mitigate uncertainty in decision-making. For example, Kennedy and O'Hagan hybrid models[92] can quantify the epistemic (model-form) uncertainty from simplifications in multiscale models[93,94]. We argue that Bayesian inference methods, which interpret probability as a belief, are conceptually aligned with stochastic and chance-constrained programming, which optimize over a probability distribution, i.e., the posterior from Bayesian model calibration. In contrast, frequentist statistical methods interpret probability as long-term error rates. Frequentist methods output confidence regions conceptually aligned with uncertainty sets for robust optimization. This perspective helps align the foundations of the data science and ML methods used to characterize uncertainty with the choice of optimization under uncertainty paradigm. Computational tractability remains a significant challenge to incorporating uncertainty in multiscale simulation and optimization problems. ML facilitates improved decomposition methods[95], aggregation and clustering[96], and branching strategies[97]. New generative AI methods are emerging to either accelerate or replace classical mixed integer optimization algorithms, e.g., fast sensitivity analysis[98].

Finally, generative AI can accelerate the problem formulation and time to solution. For example, generative AI for flowsheet synthesis[99] can dramatically reduce the time to screen novel materials (e.g., new catalyst) in the context of a chemical manufacturing process. Likewise, generative AI can propose model reformulations, variable and constraint scaling, and initialization to improve model diagnostics[100,101] to reduce the barriers to nonlinear

optimization. These advances would make sophisticated optimization paradigms more accessible to general chemical engineering practitioners instead of highly specialized experts.

CONCLUDING REMARKS

AI and ML improve the tractability of multiscale optimization, use data more effectively to quantify and mitigate uncertainty, and facilitate automation and faster time to solutions. These new capabilities complement recent trends in modeling software[102] that enable process systems engineers to guide the development of novel molecules, materials, devices, processes, and systems to address global grand challenges such as sustainable development. AI and ML provide methods that help facilitate bidirectional feedback across diverse scales and disciplines[2]. The described themes and opportunities are broadly relevant to sustainability challenges beyond the four motivating examples, such as recycling plastics, remediating legacy pollutants (e.g., perfluoroalkyl and polyfluoroalkyl substances (PFAS), lead), and decarbonizing chemical production (e.g., H_2, ammonia, biofuels).

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