Hydrogen with Carbon Management:

Roles for Artificial Intelligence in Support of FECM RDD&D Priorities

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Fossil Energy and Carbon Management

Artificial intelligence (AI) holds the potential to accelerate the transition to a carbon-neutral economy and help achieve the technology research, development, demonstration, and deployment (RDD&D) goals set forth by the DOE Office of Fossil Energy and Carbon Management (FECM) in its Strategic Vision. FECM and the National Energy Technology Laboratory (NETL) continuously expand, maintain, and curate extensive scientific data sets and AI tools essential to carbon management, and they are now standing up a robust AI Multi-Cloud Infrastructure to enable the DOE research community to share and leverage a collection of tailored resources to expedite progress toward equitable and sustainable solutions.

As one step toward prioritizing AI development activities, FECM is exploring specific roles for AI in meeting the top RDD&D needs identified in the Vision. This document summarizes a series of discussions in which a range of specialists from FECM, NETL, and the DOE Office of Science suggested potential roles for AI in **Hydrogen with Carbon Management**. This document should be viewed as a representative sample of the types of AI applications that may be needed; it is by no means a comprehensive list.

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AI for Hydrogen with Carbon Management: Summary

DOE's Hydrogen Earthshot aims to lower clean hydrogen costs 80% to $1 per kilogram within one decade while expanding the U.S. energy workforce. FECM's Hydrogen with Carbon Management (HCM) Program is building a path to achieve this Earthshot while cutting associated life-cycle greenhouse gas emissions (including methane) by 90% (DOE/FECM).

> **Hydrogen with Carbon Management**
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> "…invest in RDD&D for hydrogen production coupled with CCS using sustainably sourced carbon-based feedstocks (e.g., biomass, fossil fuels and plastics, including wastes). FECM will invest in the advancement and utility-scale demonstration of hydrogen supply and utilization technologies like hydrogen storage, reversible solid oxide fuel cells (SOFCs) and 100 percent hydrogen-fired turbines, supporting DOE's Hydrogen Shot target."
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> *FECM Strategic Vision* (DOE/FECM 2022)

The most economical ways to generate clean hydrogen today rely on fossil sources and sustainable biomass—combined with carbon capture and storage (CCS). Within the broader, DOE-wide Clean Energy Portfolio, the HCM Program supports the RD&D of new technologies for the production (with applied CCS), transport, and storage of *carbon-based* hydrogen *and* the utilization of clean hydrogen from any source. FECM's Hydrogen with Carbon Management RD&D portfolio pursues advancements in gasification; reversible solid oxide fuel cells; turbine technologies; and enabling materials, sensors, and controls.

Hydrogen is the lightest and second smallest element on earth and has the highest energy per mass of any fuel, but its volumetric energy density is extremely low at ambient temperatures. To increase this density for efficient storage and transport, hydrogen is commonly stored as a gas in high-pressure tanks (350–700 bar [5,000–10,000 psi]). For high-value applications, hydrogen can be stored as a liquid when cooled to nearly −253°C (-423°F). It may also be stored on the surfaces of solids (by adsorption) or within solids by absorption (DOE/EERE FC a).

> "Hydrogen, the second-tiniest of all atoms, can penetrate right into the crystal structure of a solid metal."
>
> David L. Chandler, *MIT News* (Chandler 2019)

Key challenges to widespread hydrogen use include maintaining hydrogen purity, increasing energy efficiency, minimizing permeation and leaks, reducing costs, and building a national delivery infrastructure for a range of regions and market types (e.g., urban, rural, or interstate) (DOE/EERE FC b). Hydrogen can also pose a challenge to the long-term integrity of high-strength steels, alloys, and other materials used in hydrogen gasifiers, reformers, turbines, wellheads, storage containers, and pipelines. Turbines using 100% hydrogen or ammonia have not yet been developed for utility or industrial-scale power generation, and the combustion dynamics of these carbon-free fuels differ significantly from those of natural gas. As summarized in Figure 1 and on the following pages, artificial intelligence (AI) and machine learning (ML) can support the Hydrogen Earthshot by assisting in the development of **structural *and* functional materials**, development of an **efficient infrastructure**, and improvement of **simulation-based engineering** and **control of unit operations**.

Structural Materials

Metallic alloys exposed to hydrogen can succumb to embrittlement (loss of ductility). At elevated temperatures, certain alloys may also experience high-temperature hydrogen attack, a phenomenon wherein carbides in the alloy react with the hydrogen to form methane bubbles, which degrade mechanical performance. In addition, in comparison to products of natural gas combustion, products of hydrogen combustion typically contain more water vapor, which can accelerate oxidation of the metallic alloys and

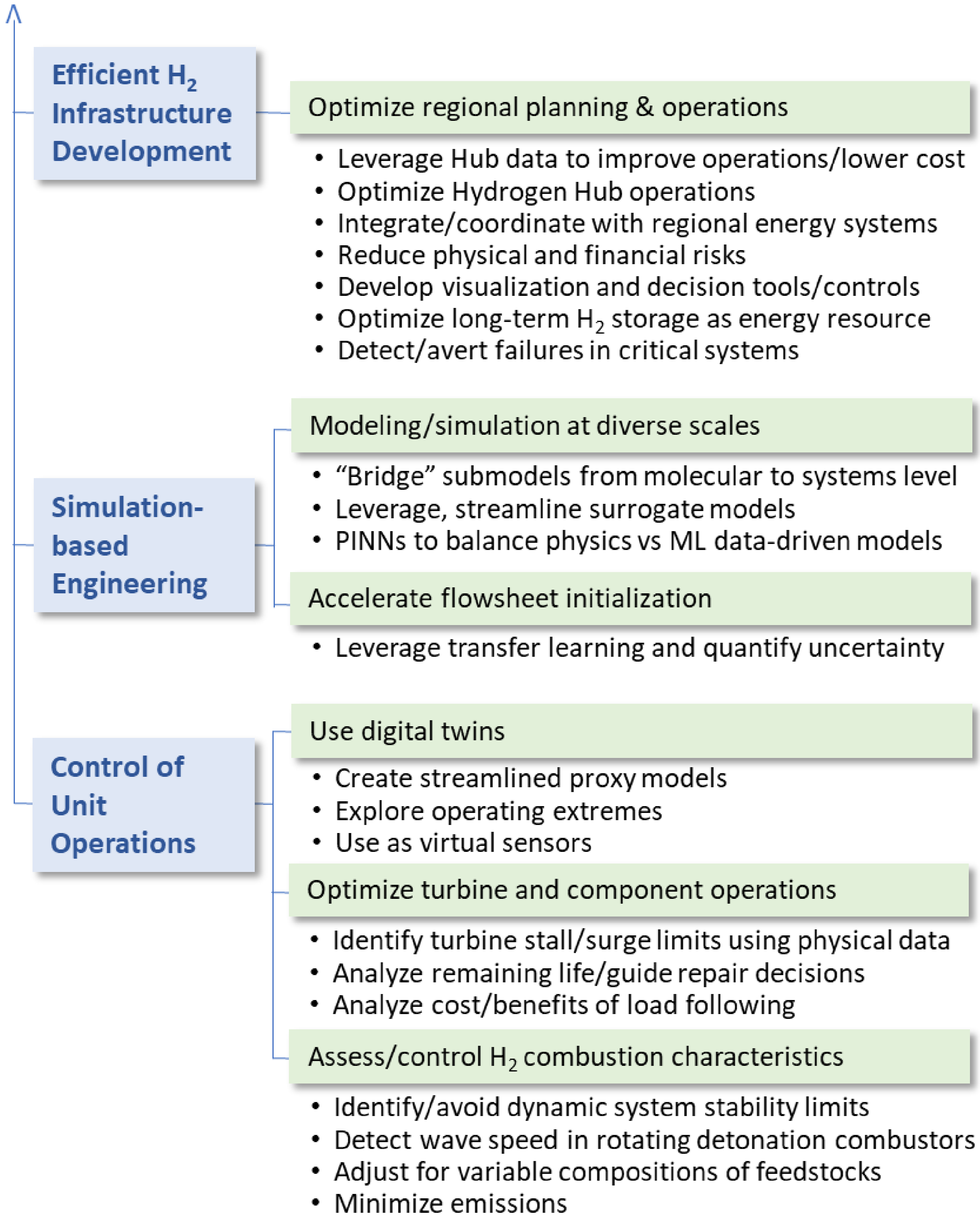
Hydrogen with Carbon Management: FECM Priority R&D with AI

Challenge — *AI Assist*

Clean Hydrogen with Carbon Mgmt.

- **Structural Materials Development**
  - Characterize materials for H_2 use cases
    - Evaluate suitability of novel materials
    - Model/predict material life/performance
    - Analyze factors in H_2 embrittlement of steels/welds
    - Analyze environments subject to H_2 trapping
    - Predict impacts of high temperatures and pressures
    - Address impacts of H_2/NG exhaust on turbines
    - Model H_2-exacerbated pipeline corrosion
  - Develop structural materials for H_2 use cases
    - Screen materials to narrow search by application
    - Improve ICME tools to formulate alloys and CMCs
    - Develop molecular-scale modeling tools (*ab initio*)
    - Advance materials processing (e.g., melt parameters
    - Reduce embrittlement factors (thermodynamics)
    - Model material degradation/microstructural changes
- **Functional Materials Development**
  - Characterize materials for H_2 use cases
    - Model material life; predict based on conditions
    - Predict degradation/changes in catalysts & cathodes
    - Image/characterize microstructures across scales
  - Develop functional materials for H_2 use cases
    - Low-temp., proton-conducting FCs and electrolyzers
    - Formulate reverse-SOFC catalysts
  - Develop oxygen-carrying materials
    - Model metal- and calcium-oxide-based O_2 carriers
    - Model condition-specific carrier performance/life
  - Enable smart components with embedded sensors
    - Assess/optimize component performance in real time
    - Detect/assess/address trends and anomalies
    - Leverage data to improve component design
    - Increase H_2 injection/withdrawal cycle efficiency

Figure 1. Summary of Potential AI Roles in Hydrogen with Carbon Management



* Physics-informed neural networks

Figure 1. Summary of Potential AI Roles in Hydrogen with Carbon Management (continued)

degrade ceramic-based environmental barrier coatings. Similarly, as the makeup of feedstocks (e.g., waste plastics, biomass) are altered during gasification, associated changes in the environment within the gasifier may degrade and corrode the refractory liner and limit service life. AI/ML methods could provide a deeper understanding of these processes in various environments, enhance efforts to characterize/predict them, and help develop novel or improved materials and coatings to resist or prevent them (FedConnect 2022).

Characterize structural materials for H_2 use cases

AI/ML tools could help assess the suitability, performance, life, and risks of **novel structural materials** (e.g., alloys, ceramic matrix composites [CMCs], coatings, embedded sensors) for use in hydrogen production, transport, and surface storage [see Methane Mitigation for geologic hydrogen storage]. AI algorithms that incorporate physical mechanisms could reduce uncertainty in the predicted performance of *new* materials and more reliably **predict the life and performance of *existing* structural materials** under specified operating conditions (including impurities).

AI could potentially draw upon recorded data (e.g., maintenance or regulatory records, operational records, and environmental/in situ data) to model impacts on the life of structural materials used in the hydrogen industry (including retrofits) under tracked conditions (e.g., temperatures, pressures, concentrations, and levels of mixing with natural gas and impurities). Areas of particular interest include embrittlement, hydrogen trapping, and the impacts of high temperatures and pressures. For example, AI might analyze the role of thermodynamics and other factors in the **embrittlement** of existing steels (and retrofits) under various hydrogen-natural gas blending schemes. AI/ML might also leverage data from advanced imaging equipment (e.g., advanced neutron scattering, atomic transmission electron microscopes, and 3D atom probe tomography) to provide useful insights on hydrogen entry, transport, and **trapping** (atomic level); molecular or elemental compositions; refractory design; predictive maintenance; and material strategies to avoid structural issues. Similarly, AI might be useful in predicting the corrosive impacts on materials subjected to hydrogen under **high temperatures and pressures** in the presence of water vapor or steam.

In addition, AI holds promise to characterize and predict the ways evolving environments and impurities affect the structural materials used in hydrogen turbines and lower-temperature hydrogen pipelines. The changing mixture of hydrogen and natural gas in a turbine affects the exhaust gas composition, water vapor content, and temperatures, all of which affect the **turbine materials** (metal alloys and coatings). AI could potentially predict those exhaust gas compositions as a function of changing conditions, predict compositions that would adversely impact the materials, and either avoid them or use them to suggest better materials. Similarly, AI might model the way a hydrogen environment exacerbates **corrosion in pipelines**, particularly in the presence of various levels of hydrogen sulfides (H_2S) and other impurities.[1]

Develop structural materials

Researchers need improved material simulation capabilities to better understand the way hydrogen diffuses into alloys and other materials, lattices, defects, and boundary interfaces (e.g., a diffusion database). A better understanding of defect energetics or how hydrogen impacts defects (e.g., dislocation, boundaries, interfaces) could clarify critical effects on materials (beyond the domain of density-functional theory) and lead to more durable materials for the hydrogen infrastructure.

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[1] Hydrogen embrittlement is a problem with high-strength, low-alloy (HSLA) steels, limiting H_2 pipelines to low-strength steel. The potential benefit of H_2-resistant HSLA steels for hydrogen compression is that less material would be needed.

AI-based tools that can identify optimal materials characteristics for a specific application would help to **screen materials** and rapidly narrow the search to expedite progress. ML methods might enhance integrated computational materials engineering (ICME) tools to help **formulate effective alloys, ceramic matrix composites**, and other novel structural materials for us in anticipated operating environments. AI models based on **elemental compositions (ab initio)** and informed by data obtained using advanced imaging equipment could perform molecular-scale analysis to improve refractory design, deliver superior performance, and provide valuable environmental benefits. AI models might also extrapolate/transfer desirable properties from the microstructural to the meso-scale. Improved models could similarly **guide materials processing** (e.g., melt parameters), **reduce embrittlement kinetics**, and **predict/prevent degradation** or corrosion. A key challenge will be the current sparsity of needed kinetic test datasets.

Functional Materials

Achieving the DOE Hydrogen Earth Shot will require a variety of novel and advanced *functional (process)* materials to optimize and lower the cost of processes used in hydrogen production, use, transport, and storage (e.g., metal hydrides that adsorb/desorb hydrogen)—and simultaneously address the degradation issues affecting structural materials (discussed above).

Characterize functional materials for H_2 use cases

AI could help characterize a range of functional materials for hydrogen use cases, including gasifiers, reformers, electrolyzers, catalysts and cathodes in fuel cells, separations membranes, and solid storage materials such as metal hydrides. AI models could predict maintenance needs, **material life**, and performance under defined operating conditions (including the presence of working fluid impurities). Models might also predict the evolution of microstructural changes in **catalysts and cathodes** in fuel cells during use and over time. Success in this area will require the availability of more long-term (>20,000 hours) stack and system test data to clarify microstructural changes, cathode poisoning, and other impacts. Finally, imaging of microstructure features (often restricted to an extremely tiny area) must scale to a useful meso level to clarify the functional impacts. AI could play a key role in **imaging across scales** and probing or characterizing the chemical environments at sites where hydrogen atoms become trapped or segregated. These imaging and scaling capabilities will support advancements in both structural and functional materials.

Develop functional materials for H_2 use cases

AI can help to develop a range of more efficient functional materials for use in hydrogen gasifiers, reformers, surface storage, fuel cells, electrolyzers, catalysts, and sensing applications. AI methods could appropriately target development of new materials (including catalysts) for more efficient, low-temperature, proton-conducting **fuel cells and electrolyzers**. For **reverse solid oxide fuel cells** (R-SOFCs), AI might provide new insights into the multi-step, complex reaction mechanisms (electrochemical and chemical) on material surfaces, interfaces, and in bulk under high temperature or high steam/partial pressure.

Develop oxygen-carrying materials

Researchers need to better understand the diffusion and degradation mechanisms in oxygen carriers to accelerate reaction times and improve both durability and cost-effectiveness. AI could help to model a range of formulations for metal oxide-based and calcium oxide-based oxygen carriers. Sufficient thermodynamic and kinetic data must first be gathered to figure out these mechanisms for individual materials, and the resulting **models of oxygen carriers** will need to be tested on alloys prior to subsequent optimization using AI. AI-based **models of carrier performance** could help to predict microstructure changes and/or degradation of oxygen carriers under a variety of anticipated operating conditions, ultimately extending carrier life and reducing costs.

Enable smart components

Sensors embedded in key components could continuously monitor and inform AI models on the performance of both structural and functional materials in the hydrogen infrastructure. In this scenario, smart components might support automated, AI-assisted, **real-time monitoring and analysis** at the component level to optimize performance, increase throughput, and lower costs. These smart components could inform and enable continuously updated AI models to analyze trends, **detect anomalies**, predict performance shifts, forecast emerging problems, and provide decision support to avert failures. AI could potentially leverage the accumulated data to diagnose issues and **improve component designs**. Insights into materials, trends, performance, and operations might then inform AI models to enable the assessment of field sites to achieve more **efficient hydrogen injection/withdrawal cycling** under various constraints.

> "… FECM funds R&D projects on carbon-neutral hydrogen pathways, including gasification, reforming, and solid oxide electrolysis cells (in coordination with HFTO [Hydrogen Fuel Cell Technologies Office], which also funds electrolysis from renewables). A specific goal of FECM is to increase carbon capture rates while lowering the cost of clean hydrogen. [FECM] also invests in hydrogen transport infrastructure; hydrogen storage; and hydrogen use for electricity generation, fuels, and manufacturing."
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> NETL Workshop Report (NETL 2021)

Efficient Infrastructure Development

Optimizing hydrogen infrastructure planning and operations should support secure, safe, and efficient hydrogen use at the regional scale. DOE's Office of Clean Energy Demonstrations (OCED) is establishing six to ten Regional Clean Hydrogen Hubs,[2] which are designed to concentrate needed hydrogen infrastructure and demonstrate economies of scale. FECM is coordinating with the offices of Energy Efficiency and Renewable Energy (EERE), Nuclear Energy (NE), Science, and other relevant DOE programs on crosscutting development efforts (e.g., demonstrations, transport, storage, industrial uses) and supports Hub activities relevant to hydrogen from fossil sources, wastes such as plastics, and available biomass, along with carbon capture and storage. The National Energy Technology Laboratory (NETL) is the clearinghouse for data collected through all Hub activities, and that data will be available to feed AI/ML tool development for all participating programs. Currently, data on and experience with regional hydrogen networks are scarce.

Optimize regional infrastructure planning and operations

AI/ML capabilities could **leverage data gathered at the Hubs** and elsewhere to suggest new ways to increase throughput, reduce costs, and/or reduce emissions at a regional scale. AI has the potential to **optimize hydrogen hub operations** and supply chains and to **integrate with the wider energy network**, expediting coordination on a regional scale. Integration of real-time data into advanced AI models could ensure timely preventive maintenance for the regional infrastructure to **reduce physical and financial risks**, provide valuable **visualization and decision tools** to balance supply and demand, and assist operators with predictive regulation and decision support. Deep learning methods and models could **optimize long-term energy storage planning** for the region, detect anomalies or vulnerabilities, and **prevent failures** in a region's pipelines, supply chains, and other critical systems. AI-enabled planning tools could provide early detection and warning capabilities,

[2] DOE's Hydrogen Hubs will connect government, hydrogen producers, consumers, and local connective infrastructure to demonstrate the production, processing, delivery, storage, and end-uses of clean hydrogen. See www.energy.gov/oced/regional-clean-hydrogen-hubs

weighted AI-informed response options, and virtual learning based on digital twins to streamline efficiency and reduce physical, financial, and environmental risks.

Simulation-based Engineering

Achieving safe, secure, efficient, clean, affordable, and integrated hydrogen energy systems will require advanced engineering tools, including sophisticated models at multiple scales.

Perform modeling and simulation at multiple scales

AI-assisted models could simulate molecular, device, or system-level phenomena within hydrogen systems *and* **"bridge" submodels across scales** to deliver useful results. AI models can continuously adapt as new data comes in, so they are particularly adept at responding in real time to evolving threats, shifts in feedstock makeup, changing operating conditions, or component degradation. The ability to **leverage ML-based surrogate models** [simplified representations of advanced simulation models to save simulation and optimization time] can help optimize system performance and reduce risk at multiple scales. Hybrid models that **merge ML and physical models** may offer the benefits of both real-world operations and adherence to the known laws of physics. For example, physics-informed neural networks (PINNs) create a balance between purely data-driven ML and physics-based models based on first principles.

A key challenge in developing accurate AI models is the limited availability of operations data to train and subsequently validate optimization models. Researchers must always reserve sufficient data to validate a model and assess its level of uncertainty for a specified application. DOE researchers can leverage NETL's capabilities to generate synthetic data for filling gaps in training datasets, curate and protect data collections, provide secure and enhanced user interfaces with data, apply transfer learning, conduct intelligent data reduction, and select specialized AI hardware to accelerate processing and simulation.

Faster flowsheet initialization

Process flowsheet initialization is often far more time consuming than solving and optimizing a model itself, creating the need for faster and more reliable initialization methods. **Transfer learning** techniques could quantify uncertainty in the generation of robust designs.

Control of Unit Operations

Some energy system operators are already using AI to accelerate data analysis and improve the quality of data synthesis to help them make complex decisions quickly (Boswell 2022). In the future, as more AI models are validated and prove their value, AI may be assigned direct control of some unit operations (Sethu 2022) to reduce human error. Significant RD&D must first prove to utilities that AI tools like artificial neural networks are sufficiently robust (and explainable) to optimize the reliability, safety, economics, efficiency, cybersecurity, and performance of energy operations.

> "There are things that took me 20 years to learn about these power plants. This model learned them in an afternoon."
>
> Lloyd Hughes, Operations Manager
> Odessa Plant, Vistra
> (Boswell 2022)

Use digital twins

Virtual copies of all system components and their interactions, known as digital twins, could help optimize hydrogen and carbon management operations. Potential applications include optimizing operating parameters in turbines, physical units, and components; characterizing, assessing, and correcting hydrogen combustion processes; and characterizing variable input (feedstock mix) and output in real time to adjust gasification parameters (e.g., temperature, pressure, oxygen flow). A validated digital twin can also train a streamlined **proxy model** that would run on a laptop (no high-performance computer needed), bringing powerful optimization and decision support tools to operators across large networks. In addition, proxy models can replace physical modeling to virtually **explore operating extremes** and the often-complex impacts of changing operating conditions or parameters. These models can virtually test potential system upgrades or responses to critical problems without putting the physical systems at risk and could assist in planning for extreme scenarios. To address the limitations of physical sensors, AI may potentially use both hybrid physical and physics-based models to **serve as virtual sensors** for the system.[3]

Optimize turbine and component operations

To improve turbine operations, AI models could use physical data to predict and recommend steps to **avoid stall or surge limits**. Another application would be to detect and **estimate the remaining life** of turbine components, then analyze the costs and benefits of replacing them (including the impacts of secondary parameters). AI might also **determine the costs and benefits of load following** (from a first principles perspective).[4]

Assess hydrogen combustion characteristics

To improve hydrogen combustion systems, AI could **identify dynamic stability limits** (flashback/blowout), anticipate when the system is approaching those limits, and recommend or take corrective action. Similarly, to provide useful diagnostics at an operations level, AI might analyze images to **detect waves and wave speeds** in rotating detonation combustors.

As gasifiers increasingly accept variable feedstocks, such as selected municipal solid wastes, AI can measure and characterize or **assess feedstock changes** in real time to recommend appropriate adjustments to the gasification operating parameters (e.g., temperature, pressure, oxygen flow rates) during operations. To help meet national carbon goals, AI might **minimize emissions** (e.g., NOx) by analyzing changes in response to ambient conditions and/or variable feedstocks.

Ultimately, AI models may replace physics-based models for hydrogen combustion, but hybrid models can combine the strengths of both in the interim: the real-time, data-driven responsiveness of AI/ML models (generally based on normal operating data) and the ability of physics-based models to suggest options for handling out-of-the-ordinary conditions.

Some Notes from the DOE Office of Science on Obtaining the Data to Drive AI

While AI thrives on data, data quality determines the usefulness of model outputs. AI has evolved to assist in collecting or generating certain types of needed data. Three options for consideration include the following:

Data digitization: AI can be informed by records originally transcribed as text or some other human-readable format (including historical data). To avoid the cost, time, and tedium of manually digitizing these records, researchers may consider using large-language models or other kinds of foundation models to process those records—with minimal use of manually tagged training data.

[3] Data obtained by physical sensors is limited by cost and environment; therefore, physics-based models can serve as virtual sensors to produce useful data. Measured (empirical) data reflect operational sweet spot (to protect system from dangerous conditions), but physics models can provide insight on wider scope of operations to develop more robust models.

[4] NETL is conducting work in this area.

Data from science-based simulations: Beyond using a broad range of recorded data, AI can take advantage of detailed scientific data produced using computational-chemistry (or other physical-based) simulations. These simulations might themselves be enhanced by AI surrogates to yield useful insights.

Data from automated labs: In cases where data needs to be gathered experimentally, a reasonable opportunity exists to use automated laboratories to systematically explore whole classes of physical experiments and collect data. DOE already has authorization to invest in automated laboratories in some areas and is open to evaluating an expanded set of use cases.

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