SSAE Newsletter

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// ABOUT

The Strategic Systems Analysis and Engineering (SSAE) directorate provides the decision science and analysis capabilities necessary to evaluate complex energy systems. The directorate's capabilities address technical, economic, resource, policy, environmental and market aspects of the energy industry. These capabilities are critical to strategic planning, direction and goals for technology R&D programs and the generation of market, regulatory and technical intelligence for NETL senior management and DOE. SSAE offers a range of multi-criteria and multi-scale decision tools and approaches for this support:

- Process systems engineering research: advanced modeling, simulation and optimization tools for complex dynamic systems
- Process and cost engineering: plant-level synthesis, process modeling and simulation of energy systems with performance estimates
- Resource and subsurface analysis: evaluation of technologies, approaches and regulations for subsurface energy systems and storage
- Market and infrastructure analysis: economic impacts and program benefits
- Environmental life cycle analysis: cradle-to-grave emissions and impacts

These tools and approaches provide insights into new energy concepts and support the analysis of energy system interactions at the plant, regional, national and global scales.

NATIONAL ENERGY TECHNOLOGY LABORATORY

// HIGHLIGHTS

Jet Fuel Production Feasible at Pittsburgh International Airport According to New SSAE Report

The feasibility of producing jet fuel from an on-site facility at the Pittsburgh International Airport (PIT) was outlined in a report by **Thomas Tarka**, Vasudev Haribal*, Stephen LeViness*, Raghubir Gupta*, Kaitlyn Fleury, **Srijana Rai***, Gregory Cooney, **Matthew Jamieson** and **Timothy Skone**. The study found that it would be technically feasible to construct and operate a gas-to-liquids (GTL) facility on PIT's property that could produce nearly 70 million gallons of synthetic jet fuel per year and supplant nearly all of PIT's current jet fuel consumption.

GTL is a commercially available technology that coverts natural gas to liquid hydrocarbons; thus, a GTL facility at PIT could convert natural gas from on-site wells to jet fuel, effectively doubling the on-site fuel stores in the event of a supply disruption. With excess production available, the GTL facility would be able to supply the U.S. Air Force Pittsburgh Air Reserve Station and 171st Air Refueling Wing, which are also at the airport.

SSAE Continues to Develop State-of-the-Art Process Modeling Capabilities

NETL's Institute for the Design of Advanced Energy Systems (IDAES) continues to advance SSAE's capabilities to design and optimize next-generation energy systems through the release of Version 1.12.0 of the IDAES Integrated Platform.

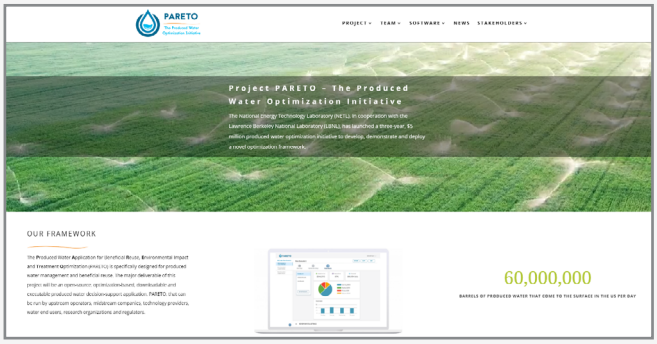
Development of this new release has been driven by the needs of several DOE projects in the areas of clean energy, hybrid energy systems and water treatment technologies.

Key new features include:

- Support for a wider range of carbon capture processes through the inclusion of a library of robust, generic models for solvent-based packed columns and ancillary equipment. Such models can be used to optimize solvent-based carbon capture from a wide range of point sources.
- New streamlined workflow for combining machine learning and artificial intelligence with rigorous process models. The workflow enables efficient surrogate model development including data collection and sampling as well as model training, verification and implementation within a single, equation-oriented programming environment.
- Improved capabilities for simulating dynamic energy systems through the integration of the PETSc library, which provides access to several numerical routines for dealing with dynamic systems and differential equations.
- Extended libraries for modeling thermophysical properties of complex systems including aqueous solutions involving electrolytes and solid-liquid equilibrium.

Project PARETO Website Launched

A new website has been launched for Project **P**roduced Water **A**pplication for Beneficial **R**euse, **E**nvironmental Impact and **T**reatment **O**ptimization (Project PARETO), a three-year, $5 million produced water optimization initiative to develop, demonstrate and deploy a novel optimization framework.



Screenshot of new PARETO website

The Project PARETO website is meant to make the initiative more accessible to a broader audience, including future stakeholders, prospective project partners and the general public. Specifically, the website offers information on the project structure and timeline, tangible deliverables, makeup of the leadership team, software download and documentation resources, as well as a section reserved for current/prospective stakeholders.

SSAE's Tarka on Team That Earns DOE Secretary's Honor Award

NETL's Multi-Functional Sorbent Technology (MUST) Team, which includes SSAE's **Thomas Tarka**, recently received the Secretary of Energy's Achievement Award for their development of a suite of sorbents that offers a practical, affordable and green approach to remove selenium and other metals that contaminate water supplies across America and jeopardize the health of millions of people, wildlife and fragile ecosystems.

This team's achievements were also recognized in October 2021 when they received a R&D 100 Award for development of this revolutionary technology. MUST is the only sorbent-based technology known to NETL that effectively reduces selenium to consistently meet federal discharge limits. Learn more.

* NETL Support Contractor

// NOTICES

SMART Produces New Models for Deep Learning

As part of the Science-informed Machine Learning for Accelerating Real-Time Decisions in Subsurface Applications (SMART) Initiative Task 5, SSAE researchers developed fast and accurate deep learning models in Python language for simulating carbon dioxide (CO_2) saturation, reservoir pressure and production rates for CO_2 storage and brine production applications. These new models were specific to a carbonate reef depositional environment in the Scurry Area Canyon Reef Operators Committee (SACROC) oil field in the Permian Basin. Historically, the SACROC oil field has been used for CO_2 injection in enhanced oil recovery application, making it an excellent candidate for studying subsurface storage of CO_2.

The model framework (Figure 1) involves assembling multi-layer autoencoder networks that provide dimensionality reduction of 3D geologic inputs with fully connected long short-term memory neural networks that generate time-series prediction of reservoir pressure, CO_2 saturation and brine production rate. This approach maximizes the training time efficiency, reduces computational memory burden and minimizes prediction turnaround.

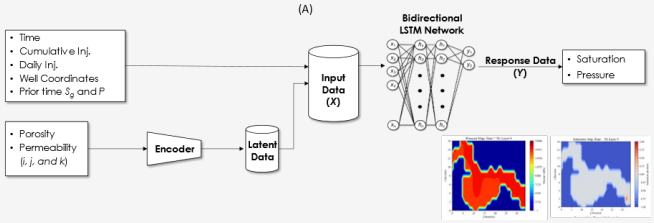


Figure 1. SMART model framework

Despite the substantially reduced dimensionality fed to the network, this framework enables minimal compromise to performance accuracy in generated models while providing extremely fast predictive turnarounds. The resulting CO_2 saturation, pressure and brine production models have accuracies greater than 99% with prediction speeds less than 1 second for one test realization of 963 timesteps covering 30 years of CO_2 injection and 100 years of post-injection periods.

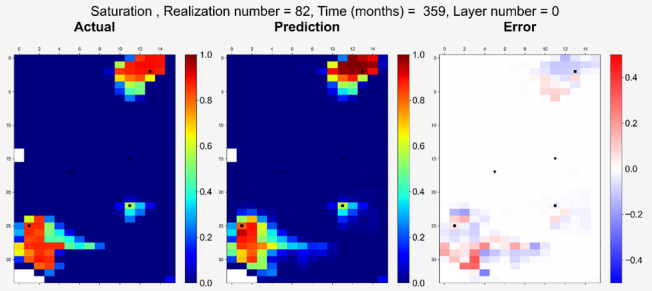


Figure 2. 3D plots of the true CO_2 saturation, predicted CO_2 saturation and the error in the top layer of a test realization of the simulated reservoir after 30 years of CO_2 injection

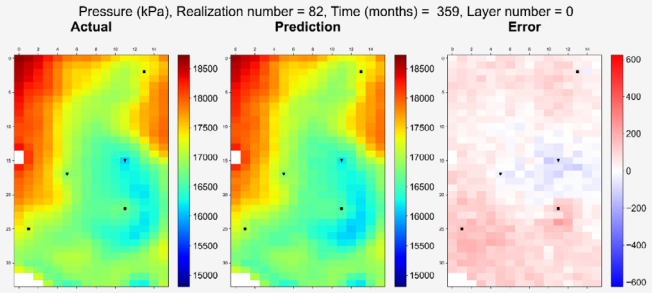


Figure 3. 3D plots of the true pressure, predicted pressure and error in the top layer of a test realization of the simulated reservoir after 30 years of CO_2 injection

Figure 2 and Figure 3 display 3D plots of saturation and pressure items, respectively, in the top layer of a test realization of the simulated reservoir after 30 years of CO_2 injection. These accuracies and prediction times point to the efficiency and utility of the models in real-world applications where model predictions are expected in a short time.

EMAT Commissions Report on Market Design for Implementation of CCS

Funded by DOE's Carbon Capture Program, SSAE's Energy Markets Analysis Team (EMAT) has engaged the National Regulatory Research Institute (NRRI) to investigate the design of market rules to incentivize the deployment of carbon capture and storage (CCS) and carbon capture, utilization and storage (CCUS), both retrofits and greenfield.

Given its close relationship with the regulatory boards, NRRI is in a unique position to advise on efficacious market design that would favor CCS deployment. Deployment of new technologies often requires specific market rules to reduce risk and enhance regulatory certainty prior to deployment. This report will outline actionable market design recommendations that could mitigate risk to CCS project developers.

AI@DOE Workshop Series

Derek Vikara* was invited to participate in the AI@DOE series of workshops, which were invite only and will conclude with a roundtable discussion on February 24, 2022. DOE's Office of Science, National Nuclear Security Administration and Applied Energy Offices, in collaboration with the Artificial Intelligence and Technology Office, have organized the AI@DOE workshops to identify artificial intelligence (AI) research requirements and priorities for the next decade. The workshop series explored areas of cross-cutting relevance, including identification of investments needed to establish a flexible environment to promote AI development and testing, partnerships to accelerate the development and adoption of AI and mission-driven needs for coordinating cross-cutting AI investments.

// NOTICES

SSAE Work to be Featured at sCO2 Power Cycles Symposium

Recent advances in supercritical CO_2 (sCO_2) power cycle technology will be presented by SSAE researchers at the 7th International sCO_2 Power Cycles Symposium, which brings together industry, academia and government agencies. SSAE work to be featured at this event, which will be held February 21–24, 2022, includes:

- A multi-staged intercooled centrifugal compressor design made for an indirect-fired sCO_2 cycle will be discussed in a presentation, "Radial Compressor Design and Off-Design for Trans-critical CO_2 Operating Conditions," by **Selcuk Can Uysal*** and **Eric Liese**.
- Development of a preliminary dynamic model for investigating the transient responses of a 660 megawatt natural gas-fueled, direct-fired sCO_2 power cycle will be highlighted in a presentation, "Dynamic modeling and simulation of a large scale direct-fired supercritical CO_2 power cycle for off-design operating conditions," by Anderson Soares Chinen* and **Eric Liese**.
- A review of spreadsheet performance and cost models of four different cooling technologies that were originally developed for indirect sCO_2 plants will be highlighted in a presentation, "Cooling System Cost and Performance Models to Minimize Cost of Electricity of Direct sCO_2 Power Plant," by **Sandeep Pidaparti***, **Charles White*** and **Nathan Weiland**.
- Investigation into the use of the partial cooling cycle as a potentially lower cost alternative to the recompression cycle for fossil-fueled power applications will be discussed in a presentation, "A Performance and Economic Comparison of Partial Cooling and Recompression sCO_2 Cycles for Coal-Fueled Power Generation," by **Sandeep Pidaparti***, **Charles White*** and **Nathan Weiland**.

System-Wide Costs of Decarbonization to be Focus of New SSAE Tools

Grid systems around the world are changing. The forefront of changes taking place are modifications to the mix of generation technologies being used to supply electricity and meet demand. Specifically, legacy power generators are being replaced with low-carbon alternatives, including variable renewable resources (VREs). VREs, however, may disproportionally increase the costs of maintaining a reliable grid system, given their need for complementary energy storage and, in some cases, the installation of capacities in excess of demand. Traditional cost metrics, such as the levelized cost of energy, fail to capture the additional costs that may be required to maintain reliability of the grid system following such changes.

Since the impact to system cost can vary depending on the characteristics of electricity markets and the corresponding suite of replacement technologies being chosen to supply electricity and meet demand, SSAE's EMAT is developing a dynamic tool based on the System Cost of Replacement Energy (SCoRE) metric for different U.S. electricity markets. The SCoRE tool estimates changes to the total system cost under scenarios where legacy carbon-intensive generators are being replaced with low-carbon alternatives, including VREs and firm generators with CCS, while still maintaining grid system reliability. The tool will aid in discerning the potential technology pathways based on appropriate combinations of VREs and CCS technologies to transition effectively to a reliable decarbonized grid with minimal system cost implications.

Subsurface Basin-Scale Modeling to be Presented at SPE Conference

"Basin Management of Geologic CO_2 Storage: Effect of Well Spacing on CO_2 Plume and Pressure Interference," will be presented by **Nur Wijaya*** at a dedicated session on CCS on April 26, 2022, at the 2022 Society of Petroleum Engineers (SPE) Western Regional Meeting. The presentation will discuss advances in modeling geologic storage of CO_2 in saline formations using a full-physics 3D TOUGH reservoir simulator. Modeling results analyzing the interactions of CO_2 plume and basin-scale pressure build-up from CO_2 injection sites potentially located in proximity will also be discussed. Concerns over both CO_2 plume co-mingling from different injection sites over the long term during post-injection site care and excessive pressure build-up that could endanger the caprock integrity or approach the maximum allowable reservoir pressure increase per the U.S. Environmental Protection Agency's Underground Injection Class VI well regulations will be highlighted. A paper discussing the analysis will also be published in the conference proceedings.

// SSAE CORE CAPABILITIES

Subsurface Energy Resource Analysis at NETL

The NETL SSAE Directorate's subsurface energy resource analysis capability provides geotechnical and engineering expertise to better understand, delineate, appraise and promote safe utilization of critical subsurface energy resources. This analysis is complex and multi-faceted, often requiring tailored evaluation strategies taking into account a resource's subsurface composition, location and end-use destination while considering factors such as environmental impact, utilization economics and available and/or emerging technologies. The varied subsurface energy resources that exist—including energy feedstocks (e.g., oil, gas, coal and geothermal), long-term storage options for captured CO_2, midstream geologic storage options that ensure timely energy feedstock supply and pay zones for critical minerals and rare earth elements—share exploration and development commonalities. However, substantial disparity exists in how these are best appraised, extracted, used and managed, depending on the intended use case. As a result, implementing holistic subsurface resource evaluation requires a highly multi-disciplinary approach leveraging science, engineering and economic principles.

Subsurface energy resource analysis supports and guides many of DOE's existing research programs and initiatives by coupling mission-space objectives associated with improving the identification and utilization of one or several subsurface energy resources. These programs, which are part of the Office of Fossil Energy and Carbon Management (FECM), include the Carbon Storage Program, Office of Resource Sustainability, SMART Initiative and NETL's Crosscutting Research Program.

The team develops analyses, data and models accommodating the scientific, engineering and techno-economic aspects needed for holistic subsurface energy resource evaluation. Both stand-alone products and those integrated into a larger energy system evaluation are critical for informing key stakeholders on subsurface energy system performance, associated cost drivers, practical research pursuit ventures, environmentally safe solutions and potential economically viable deployment options.

Subsurface energy resource analysis within SSAE is centered around four key research and analytical objectives:

1. **Subsurface energy resource identification, quantification and utilization**: Generating subsurface CO_2 storage capacity and energy feedstock resource estimates, geologic datasets and wellbore design and completion engineering tailored to in-field conditions.
2. **System behavior modeling, analysis and optimization**: Modeling geologic conditions, simulating operational aspects of CO_2 storage and enabling optimization at multiple scales (project, reservoir, basin and nationwide) with the ability to leverage data-driven machine learning (ML) approaches for predictive modeling.
3. **Resource utilization economics and policy considerations**: Performing techno-economic analyses of integrated energy systems (e.g., onshore and offshore CO_2 transport, CO_2 storage, and unconventional oil and gas [O&G] forecasting) under various economic and development scenarios, as well as supporting the creation of quality guidelines for estimation of CO_2 transport and storage cost.
4. **Programmatic strategic support and analysis**: Evaluating the opportunities, challenges and research gaps and needs implicated in the dynamic of emerging technologies (like intermediate storage of CO_2 for utilization), energy resources (e.g., methane hydrates, residual oil zones, offshore CO_2 and hydrogen), policies and regulations (like offshore O&G regulations, 45Q tax incentives and National Environmental Policy Act) and environmental impacts from capture, utilization and storage developments relevant to the evolving U.S. energy landscape.

Products are disseminated as NETL-published reports, peer-reviewed journal manuscripts and conference/event papers/presentations. Some key products include:

- Evaluating CCS value chain and financial incentives
  - » Quality Guidelines for Energy System Studies: Carbon Dioxide Transport and Storage Costs in NETL Studies
  - » Comparative Analysis of transport and storage options from a CO_2 source perspective
  - » Comparative Analysis of Carbon Capture and Storage Finance Gaps and the Social Cost of Carbon
  - » Water Management Cost Assessment of CO_2 Storage Operations
- Offshore CO_2
  - » Cognac, Petronius and Horn Mountain offshore oil field case studies
  - » Screening and Identifying High-Suitability Offshore CCUS Storage Areas in the Gulf of Mexico Using a Multi-Criteria Evaluation Approach
- ML/SMART
  - » Machine learning-informed ensemble framework for evaluating shale gas production potential: Case study in the Marcellus Shale
  - » Evaluation of Time-Step Frequency on Prediction Accuracy Applied to Deep Learning Neural Network Surrogate Models for CO_2 Storage
- CO_2 geologic storage considerations
  - » NETL's Analog Studies to Geologic Storage of CO_2 – Overview
  - » Using Geophysical Technologies Deployed in Inexpensive Monitoring Wells to Monitor the Evolution of a CO_2 Plume: Potential Benefits and R&D Needs
  - » Overview of Potential Failure Modes and Effects Associated with CO_2 Injection and Storage Operations in Saline Formations

// SSAE CORE CAPABILITIES (cont'd)

- Hydrocarbon and/or CO_2 storage resource assessments
  - » Four-county San Andres
  - » Eight-county San Andres
  - » Evaluation of Technically-recoverable resources in the Marcellus and Utica shale gas plays of the Appalachian basin

Additionally, SSAE's subsurface energy resource analysis publishes open-source CCUS models designed to help effectively evaluate CCUS costs at each link in the value chain. These models can be used independently or in conjunction with each other:

- FECM/NETL CO_2 Transport Cost Model (CO2 T COM)
- FECM/NETL CO_2 Saline Storage Cost Model (CO2 S COM)
- FECM/NETL CO_2 Prophet Model
- FECM/NETL Onshore CO_2 EOR Cost Model (CO2 E COM)

SSAE's subsurface energy resource analysis capability is critical to understanding the complex nature of the subsurface, helping define programmatic goals and objectives and advancing research. Efforts are essential to ensuring a safe and sustainable energy future that aligns with NETL and DOE missions. – Contributed by **Travis Warner*** and **Derek Vikara*** in support of SSAE's Energy Systems Analysis Team

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// UPCOMING

SSAE Federal staff and NETL support contractor personnel will attend or present at the following conference and events in February 2022:

- 2022 Produced Water Society Seminar
  Presenters: **Miguel Zamarripa-Perez*** and **Andres Calderon***
  Houston, TX, February 8–9, 2022
- Carbon Capture, Transport and Storage Workshop during 2022 Produced Water Society Seminar
  Presenters: John Litynski (DOE-HQ), **David Miller (DOE-NETL)**, Dustin Crandall (DOE-NETL), **Markus Drouven (DOE-NETL)** and Lisa Henthorne (DOE-Lawrence Berkeley National Laboratory)
  Houston, TX, February 9, 2022
- EPRI Generation Advisory and Council Meetings
  Participants: **Thomas Tarka**, **Eric Grol** and **Timothy Fout**
  Hybrid (Virtual and Scottsdale, AZ), February 14–18, 2022
- 7th International sCO_2 Power Cycles Symposium
  Presenters: **Selcuk Can Uysal***, Anderson Soares Chinen* and **Sandeep Pidaparti***
  Participant: **Nathan Weiland**
  Hybrid (Virtual and San Antonio, TX), February 21–24, 2022

// CONFERENCES AND EVENTS

- 2022 Produced Water Society Seminar
  Houston, TX, February 8–9, 2022
- EPRI Generation Advisory and Council Meetings - February 2022
  Hybrid (Virtual and Scottsdale, AZ), February 14–18, 2022
- 7th International Supercritical CO_2 Power Cycles Symposium
  Hybrid (Virtual and San Antonio, TX), February 21–24, 2022

// RECENT PUBLICATIONS

Reports

A. DeMordaunt, **S. Sharma***, **M. Stypula***, **C. Charlton*** and S. Lin, "Market Analysis: Upcycling Natural Gas into Solid Carbon Products," National Energy Technology Laboratory, DOE/NETL-2021/3211, Pittsburgh, PA, March 24, 2021.

T. Tarka, V. Haribal*, S. LeViness*, R. Gupta*, K. Fleury, **S. Rai***, G. Cooney, **M. Jamieson** and **T. Skone**, "Jet Fuel Production at the Pittsburgh Airport: GTL Via Fischer-Tropsch Synthesis," National Energy Technology Laboratory, DOE/NETL-2021/2853, Pittsburgh, PA, December 2, 2021.

A. Zoelle, **T. Schmitt***, **S. Homsy***, **M. Woods***, **T. Shultz**, **T. Fout** and J. Hoffmann, "Bituminous Coal and Natural Gas to Electricity: >90% Capture Cases Technical Note," National Energy Technology Laboratory, DOE/NETL-2022/3222, Pittsburgh, PA, December 30, 2021.

Conference Proceedings and Events

E. Hedrick, K. Reynolds, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Development of Algorithms for Reinforcement Learning Augmented Model Predictive Control," presentation at the 2021 American Institute of Chemical Engineers (AIChE) Annual Meeting, Boston, MA, November 8, 2021.

K. Reynolds, E. Hedrick, **B. Omell**, **S. Zitney** and D. Bhattacharyya, "Dynamic Optimization of the Operational Trajectory of a Supercritical Pulverized Coal-Fired Boiler Under Load-Following with Consideration of Boiler Health," presentation at the 2021 AIChE Annual Meeting, Boston, MA, November 10, 2021.

E. Hedrick, K. Reynolds, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Nonlinear Predictive Control of an Industrial Selective Catalytic Reduction Unit," presentation at the 2021 AIChE Annual Meeting, Boston, MA, November 10, 2021.

E. Hedrick, K. Reynolds, S. Hong, D. Bhattacharyya, **S. Zitney** and **B. Omell**, "Advanced Model Predictive Control for Reducing Equipment Damage in a Supercritical Pulverized Coal Fired Power Plant during Load-Following Operation," presentation at the 2021 AIChE Annual Meeting, Boston, MA, November 11, 2021.

K. Reynolds, E. Hedrick, **B. Omell**, **S. Zitney** and D. Bhattacharyya, "Health Monitoring of an Industrial Supercritical Pulverized Coal Boiler," presentation at the 2021 AIChE Annual Meeting, Boston, MA, November 11, 2021.

* NETL Support Contractor

// REFERENCE SECTION

Models / Tools / Databases

- FE/NETL CO_2 Transport Cost Model
- FE/NETL CO_2 Storage Cost Model
- FE/NETL CO_2 Prophet Model
- FE/NETL Onshore CO_2 EOR Cost Model
- Life Cycle Analysis Models
- NETL LCA CO2U toolkit
- IDAES Power Generation Model Library
- Pulverized Coal Carbon Capture Retrofit Database (CCRD)
- Natural Gas Combined Cycle CCRD
- Industrial Sources CCRD

Key Reports

- Baseline Studies for Fossil Energy Plants
- Quality Guidelines for Energy System Studies
- Life Cycle Analysis

- SSAE website
- Search for other SSAE products
- Institute for the Design of Advanced Energy Systems webpage
- Life Cycle Analysis webpage
- $CCSI^2$ webpage

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