



Artificial Intelligence in Carbon Capture, Utilisation and Storage 2025 Workshop

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IEAGHG

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IEAGHG are at the forefront of cutting-edge carbon, capture and storage (CCS) research. We advance technology that reduces carbon emissions and accelerates the deployment of CCS projects by improving processes, reducing costs, and overcoming barriers. Our authoritative research is peer-reviewed and widely used by governments and industry worldwide. As CCS technology specialists, we regularly input to organisations such as the IPCC and UNFCCC, contributing to the global net-zero transition.

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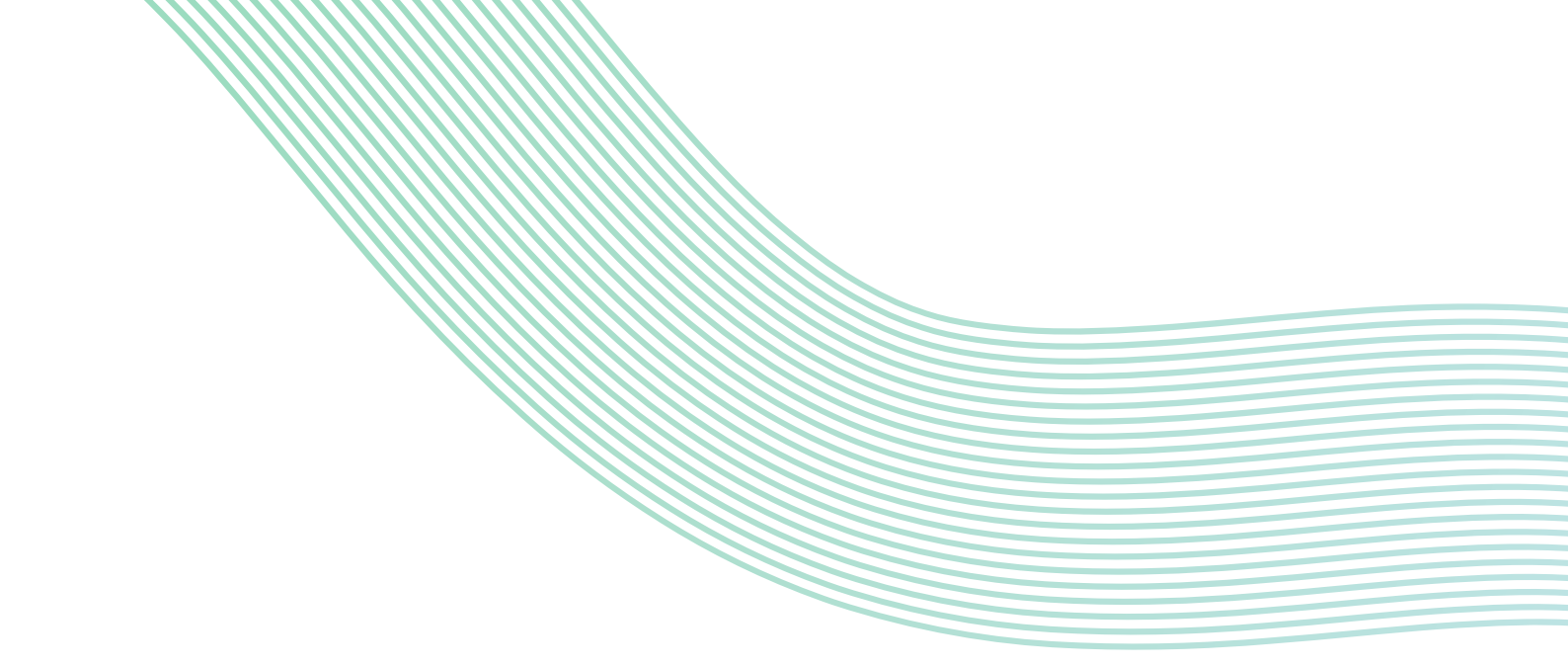
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Executive Summary

The IEAGHG AI in CCUS Workshop, held virtually on 29–30 April 2025, was convened to foster a deeper understanding of the role artificial intelligence (AI) can play in advancing carbon capture, utilisation and storage (CCUS). The first day, with 266 attendees, focused on fact-finding: reviewing the present status of AI applications across the CCUS value chain and show-casing case studies that demonstrate both the capabilities available today and the potential AI holds for the near future. The second day shifted towards interactive, collaborative discussions with 43 invited experts, aimed at unpacking the risks, opportunities, and barriers associated with integrating AI into CCUS operations. Through this process, the workshop sought to identify research gaps and recommendations for addressing them.

The conclusions from both days include:

- AI is a transformative enabler for CCUS, i.e. has demonstrated significant potential to accelerate innovation, improve operational efficiency, and reduce costs.
- Real-world applications are emerging, enhancing material discovery, automating subsurface analysis, streamlining permitting, and monitoring CO₂ transport and storage.
- Trust, transparency, and explainability are critical, thus applications require models that are interpretable and auditable. Black-box systems face resistance, especially in permitting and public engagement.
- Data remains a major bottleneck. High-quality, diverse, and standardised datasets are essential for training robust AI models. Lack of these will likely lead to increased hallucinations.
- AI should augment—not replace—human expertise. Across all sessions, participants agreed that AI must support human decision-making rather than automate it entirely.
- Environmental and ethical considerations must be addressed. The energy intensity of AI models, potential biases, and risks of overreliance were highlighted as concerns.

Following on, we recommend the actions below to overcome the concerns identified above:

- Establishment of cross-sector data sharing frameworks between industry, academia, and government to unlock proprietary and siloed data.
- Investment in explainable and interpretable AI to ensure model transparency from the development phase.
- Development of benchmarking and validation protocols and alignment of AI validation with traditional engineering and scientific methods.
- Supporting interdisciplinary training and capacity building, i.e. training CCUS professionals in AI and vice versa.

- Accelerating permitting with AI tools to reduce review times and associated costs and improve completeness checks.
- Promotion of energy-efficient AI development by e.g. developing low-power models and investing in low-carbon energy-powered data centres.
- Embedding AI into digital twins and monitoring, reporting and verification (MRV) systems to enhance real-time monitoring, predictive maintenance and carbon credit issuance.
- Alignment of AI deployment with evolving policy frameworks, such as the EU AI Act and Article 6 of the Paris Agreement.

Introduction

The IEAGHG AI in CCUS Workshop, held virtually on 29–30 April 2025, was convened to foster a deeper understanding of the role artificial intelligence (AI) can play in advancing carbon capture, utilisation and storage (CCUS). The workshop brought together researchers, industry and professionals to explore current developments, identify emerging challenges, and shape future directions at the intersection of AI and CCUS.

The first day focused on fact-finding: reviewing the present status of AI applications across the CCUS value chain and showcasing case studies that demonstrate both the capabilities available today and the potential AI holds for the near future. The second day shifted towards interactive, collaborative discussions aimed at unpacking the risks, opportunities, and barriers associated with integrating AI into CCUS operations.

Through this process, the workshop sought to identify research gaps and strategic recommendations for addressing them. The outcome is to define the 'grand challenges' in this evolving field and to generate insights that are actionable and valuable for researchers, the broader CCUS community and funding organisations.

Welcome Remarks

The IEAGHG AI in CCUS Workshop opened with a warm welcome from **Jasmin Kemper** (IEAGHG), who thanked participants for joining and introduced the purpose of the event. She emphasised that the workshop aimed to build understanding around the role of AI in CCUS, with a focus on reviewing the current landscape, highlighting real-world applications, and fostering discussion on future opportunities. Jasmin also noted the importance of fact-based dialogue supported by case studies from invited experts actively integrating AI into their work.

Following the welcome, **Abdul’Aziz Aliyu** (IEAGHG) provided an introductory overview of IEAGHG, outlining the organisation’s mission, key activities, and ongoing work programme and highlighted the collaborative nature of the workshop in exploring cross-cutting themes between AI and CCUS.

Keynote Remarks: Opportunities and Challenges of AI in Carbon Capture and Storage

Julio Friedmann (Carbon Direct) opened the workshop with a timely and engaging keynote that introduced the growing role of AI in advancing CCUS, drawing on insights from the Innovation for Cool Earth Forum (ICEF) AI Roadmap¹. He highlighted that AI is increasingly driving progress across the CCUS value chain by enabling capabilities such as detection, prediction, optimisation, and simulation.

He outlined seven key areas where AI can accelerate the deployment of CCUS technologies. In material discovery, AI enables the rapid identification, screening, and optimisation of novel sorbents, solvents, and electrocatalysts. It also supports reactor design by conceptualising more efficient systems for CO₂ capture and conversion. In facility operation and retrofit, AI-driven monitoring and digital twins enhance performance, fault detection, and retrofit planning.

Furthermore, AI contributes to transport optimisation by improving pipeline routing and multimodal CO₂ transport including rail, barge, and truck while accounting for cost, environmental, and social factors. For storage site characterisation and operation, AI aids in greenfield site screening, subsurface modelling, and monitoring. It also supports permitting and oversight by streamlining regulatory review, facilitating public engagement, and informing policy decisions. Finally, in non-technical enablement, AI enhances communication and transparency, helping to build community acceptance and more effectively predict potential impacts.

Julio emphasised the importance of high-quality, accessible data for training effective AI models, cautioning against risks such as data bias, hallucinations in generative models, and policy over-reliance on unvalidated AI outputs. He strongly advocated for workforce training, interdisciplinary collaboration, and the appointment of dedicated AI officers within climate and energy agencies.

Importantly, Julio noted that while AI can enable CCUS, CCUS can also enable AI, particularly in decarbonising data centres and power systems that support the growing AI infrastructure. He cited emerging industry interest from companies such as Meta and Chevron, describing CCUS as a "decarbonisation backstop" for AI-driven developments.

He concluded by urging stakeholders to look beyond incremental improvements and instead harness AI for "curve-jumping" innovation technologies that fundamentally shift performance and efficiency boundaries.

¹ <https://www.icef.go.jp/roadmap/>

Session 1: Generative AI and high-performance computing for the accelerated discovery of materials for energy storage and conversion

Eliu Huerta (Argonne National Laboratory) presented MOFA, a generative AI framework based on a molecular diffusion model for the design of metal–organic frameworks (MOFs) targeting both carbon capture and energy conversion applications. MOFA combines AI-designed organic linkers with specific metal nodes to generate synthesizable and structurally valid MOF candidates. These are rigorously screened using molecular dynamics, density functional theory, and Monte Carlo simulations to assess their stability, chemical consistency, and CO₂ adsorption performance. In a recent breakthrough, MOFA identified six novel MOFs that outperformed 96.9% of existing MOF datasets in adsorption capacity, demonstrating the transformative potential of AI for accelerating material discovery across both carbon management and energy storage domains^{2,3}.

Eliu also introduced new capabilities integrated into the MOFA workflow, including the use of gRASPAs to study material performance in the presence of moisture a critical factor for real-world CO₂ capture. Notably, computations that previously required days using RASPA can now be completed in minutes with gRASPAs, significantly accelerating the screening process. The MOFA workflow has also been successfully deployed on Aurora, one of the world's most powerful exascale computing systems, enabling rapid evaluation of thousands of MOF candidates and reinforcing AI's potential to transform materials discovery at scale.

Looking ahead, the MOFA framework is progressing toward practical deployment through a staged roadmap. In the short term, efforts are bearing fruit since a handful of high-performance MOFs have been synthesised and validated at Argonne's Materials Engineering Research Facility (MERF). In the medium term, the goal is to identify scalable materials with strong potential for commercialisation. In the long term, the vision is to spearhead advances in AI, including autonomous discovery labs, quantum computing, and the future use of zetascale computing to accelerate materials innovation at unprecedented scales.

² Park, H., Yan, X., Zhu, R. *et al.* A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture. *Commun Chem* **7**, 21 (2024). <https://doi.org/10.1038/s42004-023-01090-2>

³ Yan, X., Hudson, N., Park, H., Grzenda, D., Pauloski, J. G., Schwarting, M., ... & Huerta, E. A. (2025). MOFA: Discovering Materials for Carbon Capture with a GenAI-and Simulation-Based Workflow. *arXiv preprint arXiv:2501.10651*.

Session 2: AI in CO₂ Storage – Examples from Shell

Jeroen Snippe (Shell) delivered an overview of emerging applications of AI in CO₂ storage, drawing on real-world use cases from Shell's portfolio. Jeroen's presentation was structured around three main themes: plume migration prediction, legacy well data integrity assessment, and monitoring data analysis. Across these domains, AI was shown to offer significant potential in reducing project cycle time, improving operational efficiency, and supporting the scale-up of CO₂ storage to gigatonne levels.

For site capacity and containment screening, Jeroen presented a surrogate modelling approach aimed at enabling rapid CCS site screening. The AI-driven tool is designed to make dynamic CO₂ plume modelling more accessible and practical during early-stage site assessments, with high accuracy. Future developments are focused on reducing the computational burden of this modelling through enhancements to the Fourier Neural Operator (FNO) architecture and adapting it to handle complex geological features such as non-flat top surfaces, faults, and varying injection locations.

In the area of well integrity, Jeroen highlighted the time-intensive challenge of reviewing legacy well data and preparing associated diagrams manually. To address this, Shell has developed a digital tool powered by Optical Character Recognition (OCR), Natural Language Processing (NLP), and Machine Learning (ML). This tool enables automated extraction of key well information, produces one-click well status and plumbing diagrams, and provides a centralised platform for storing evaluation results. The solution significantly streamlines workflows, preserves institutional knowledge, and supports more consistent, accessible decision-making across teams.

For operational monitoring, the presentation focused on Shell's risk-based Measurement, Monitoring, and Verification (MMV) approach. This framework uses a bowtie risk structure to treat monitoring as an active barrier, ensuring that risks are effectively mitigated throughout all phases of storage operation. The monitoring system is adaptable, evolving with updated risk assessments, and is designed to achieve multiple goals: demonstrate containment and conformance, support emissions accounting, provide evidence for stakeholder assurance, and facilitate the eventual transfer of long-term liability.

Finally, Jeroen introduced a ML-based anomaly detection workflow using Distributed Temperature Sensing (DTS) data from the Quest CCS project. The approach was tested on pseudo-empirical datasets combining field data with synthetic anomalies and showed sensitivity to temperature deviations as low as 0.5°C in targeted geological layers. The random forest algorithm was identified as the preferred model, and the workflow has now been deployed across three injection wells, with ongoing testing over a period exceeding one year. These results demonstrate the practical viability of ML tools in enhancing real-time subsurface monitoring.

Session 3: Transforming Subsurface Analysis with Advanced AI and Machine Learning Techniques

Athanasios (Athos) Nathanail (Colorado School of Mines) presented on the application of advanced AI and ML techniques to significantly enhance the speed, accuracy, and automation of subsurface geological analysis, with a focus on CCS and mineral exploration. He highlighted the use of technologies such as generative AI, computer vision, and convolutional neural networks (CNNs) to improve seismic imaging resolution, generate synthetic datasets, and interpret depositional environments. By integrating multi-scale geological data from outcrops, cores, and seismic surveys, this AI-driven approach aims to reduce uncertainty in CCS site characterisation and improve the precision of identifying economically viable mineral deposits.

Athos outlined several key challenges facing traditional subsurface interpretation. These include the overwhelming volume and complexity of data, difficulties in bridging scales between different data types, the labour-intensive nature of geological interpretation, and the uncertainty and subjectivity that arise from incomplete or noisy data. Siloed analysis of textual reports, imagery, and sensor data further limits the ability to see the full geological picture.

AI and ML were presented as powerful tools to overcome these barriers, offering capabilities in rapid pattern recognition, consistency in interpretation, and the ability to manage complex, multi-dimensional datasets. Applications relevant to CCUS include site characterisation, monitoring and surveillance, risk assessment, data-driven insight generation, training, and permitting. One of the project's goals is to build an AI system capable of automating the interpretation of depositional environments from outcrop imagery, including the ability to quantify uncertainty and transfer insights across scales.

A particularly promising area discussed was the use of generative AI for seismic imaging. Using stable diffusion methods, the model can enhance low-quality seismic data, generate synthetic seismic sections for areas with sparse data, and create training datasets for other machine learning models. These AI-driven capabilities support more accurate, consistent, and scalable seismic analysis.

Athos concluded by underscoring AI's transformative role in subsurface analysis. He emphasised that interpreting depositional environments remains central to understanding rock properties and fluid behaviour, and that AI acts as a catalyst for integrating field, laboratory, and geophysical data into more robust geological models. By quantifying uncertainty and enabling real-time model updates, AI can help reduce key exploration and CCS risks such as drilling non-viable injection wells ("dry wells") or overlooking potential leakage pathways thereby improving decision-making and confidence in site selection. Looking ahead, further advances in AI, particularly in

explainability, real-time data integration, and physics-informed learning, will continue to strengthen collaboration between geoscientists and intelligent systems.

Session 4: AI-Informed Risk Assessment for CCUS

Ken Hnottavange-Telleen (GHG Underground LLC) presented on AI-informed risk assessment for CCS and CCUS projects, with the aim of AI augmenting, not replacing, human experts. Asking ChatGPT about the topic, there are three main challenges that ChatGPT currently cannot do directly: (1) access confidential or proprietary project data, (2) perform quantitative risk calculations autonomously, and (3) make final risk judgements without human oversight. Ken quoted recent findings from researchers at Johns Hopkins University, showing the inability of 350 current AI models to consistently decipher nonverbal cues in human communications, i.e. being unable to 'read the room'.

Ken then provided the essential definitions used in risk assessment for CCUS, such as project values, scenarios, likelihood scale and severity scale, highlighting that for the latter, only humans can define and weigh these. AI models and human subject matter experts (SMEs) share that both have biases, so a lot of effort goes into how to minimise them, e.g. assembling a sufficient number of human experts from a diversity of relevant backgrounds and subjecting them to live discussions. A distinguishing feature between AI models and human experts is that the latter rarely hallucinate in public. AI can however potentially supplement the human exchange by providing immediate curated and proprietary data.

When deciding to gauge whether to use AI tools for risk assessment, it is important to keep the following assertions in mind. CCUS projects, especially first-of-a-kind (FOAK) ones, rely on sparse, often imprecise data. Secondly, only humans can weigh disparate values and judge the importance of unknowns. And lastly, SMEs and stakeholders are the best qualified to identify reliable sources/data. So, in conclusion, AI should only be used as a supplement to best inform the human experts who make the final risk judgements, as the principle 'garbage-in-garbage-out' (GIGO) still applies to AI models.

Ken then proceeded to discuss how AI can aid CCUS project risk assessment in particular, noting that this might change in the future as AI models change. One advantage of AI is that it can often offer vast curated base of known and forgotten information, which might include proprietary data. Thus, it can provide information 'at experts' fingertips' for use pre- or during discussions. It remains to be seen though, whether AI tools can yield consistent risk quantification across multiple projects.

Session 5: Use of AI with Respect to Biomass Origin and Tracking

Phil Brightman and Simon Herzberg (Drax) presented on how Drax AI to ensure the sustainability of the biomass they are using. Simon started by explaining how satellite remote sensing data in combination with AI can be used to improve and automate processes in relation to forest harvesting and carbon sequestration. Drax doesn't harvest biomass itself, so AI tools can help to verify sustainability claims of existing and onboarding suppliers.

Phil elaborated more on how the AI is used to identify harvest locations and times with satellite imagery. AI enables more precise and less time-consuming identification of harvested areas. Combining this with technologies such as LIDAR and near-infrared, vegetation cover can be estimated and compared against publicly available dataset on deforestation, forest fires, pests and diseases to flag areas of potential carbon loss for investigation.

Simon then provided an example of how AI image analysis is more accurate than human hand-drawn polygons, especially when identifying exclusion areas. Phil added that AI is also better at spotting pixel level changes across large numbers of locations, which helps with identifying land use changes more quickly and accurately. This can then be flagged for human cross-check and verification, reinforcing messages of earlier speaker that AI should assist, not replace human experts.

The tools presented can also be used for improving active forest and carbon stock management, with newer, recently launched satellites being able to better deal with obstructions such as cloud cover and canopy. Phil finished with mentioning that another area that will be of increasing importance besides satellite data analysis is the integration of other data sets, e.g. on biodiversity. Simon added a closing remark that the time-savings provided by AI-assisted analysis have already made the job of the sustainability team at Drax much more efficient.

Session 6: AI Use Cases for CCUS Permitting

Eric Redmond (ClassVI.ai) started his talk also emphasising that AI is not a replacement for human judgement, that using AI tools is not about mere automation but acceleration. He then highlighted that energy permitting delays can severely curb decarbonisation effort. Taking Class VI permits as an example, the US Environment Protection Agency (EPA) permit approval timeline is aimed at 24 months but currently can take an average of 44 months, leading to billions of USD lost in clean energy investments, GDP and NVP.

Class VI permits can easily reach over 20k pages, taking human significant time to review. AI can help by significantly speeding up the process during almost all steps of the process, especially the completeness review, response to notices of deficiency, the technical review and the response to requests for additional information. However, data management and data governance are just as important as using advanced tools like AI.

Eric then pointed out the types of AI that are relevant for use in permitting, i.e. Natural Language Processing (NLP), including Large Language Models (LLMs) but also Small Language Models (SLMs) and Optical Character Recognition (OCR), classifiers and neuro-symbolic AI (NSAI), which is a form of AI that leverages neural networks but codifies into first-order logic, helping with explainability and addable, making it easier to see for the user whether the AI makes logical conclusions. In permitting, AI can also be used as a general-purpose learning tool, as writing and reviewing permits draws on a broad set of expertise. In this regard, AI could help with quickly communicating thoughts and ideas, learning new uses, and add structure to new areas of exploration.

Next, Eric discussed some of the issues that are related to adopting the use of AI in permitting and how to alleviate them. These include the accuracy and completeness of technical information, otherwise hallucinations are likely to occur, and current research is indicating that by feeding more data into AI models, the error rates and hallucinations are growing, rather than decreasing as hoped. This can be countered by using models are not or less prone to hallucination, such as NSAI. Another issue are regulatory and legal compliance risks, as regulation can be driven by preference and/or implicit/tacit knowledge. Thus, capturing this implicit/tacit knowledge should be a core feature of designing the AI model/tool. Then there is potential human credulity in the case of an AI that appears extremely confident, which can lead to humans bypassing cross-checking and validating the outputs of AI models. This could be improved by increasing the explainability and auditability of the AI, creating feedback loops that prioritise attention. On top of that, there can be questions regarding the data quality and availability that the AI uses and is trained on, which can often be sparse, incomplete, biased and/or unstructured. These issues are very hard to fully alleviate but this underlines again that a core feature in developing AI tools should be conscientious data acquisition, management and governance. Lastly, the energy intensity of training and using AI models could ultimately be counterproductive to the goal of reducing carbon emissions. Thus, looking into lower power models like SLMs and low-carbon energy supply options is crucial.

Eric summarised his talk by reiterating that AI can be a tool to accelerate permitting (not just in the CCS space but also in other industries) but that humans should focus on making the critical decisions.

Session 7: Advancing CCUS with Generative AI: Agent George and The Open Footprint Data Model

Jon Curtis and Bertrand Rioux (Petrolink/Net Zero Matrix) presented on how to advance the CCUS supply chain with generative AI, using the tool Agent George, the Open Data Footprint Data Model and the OSDU Data Platform.

Jon started by explaining that for efficient CO₂ geological storage, we will need high quality geotechnical planning data, which includes quantification of trap and seal risk. Later, CO₂ containment needs to be ensured by rigorous geotechnical monitoring, reporting and verification (MRV). Data quality and security related to carbon accounting is a main concern for multiple stakeholders, i.e. project operators, regulators and the public. This is even more important for CCUS shared T&S infrastructure, and for monetisation third-party independent validation will be required.

The Open Subsurface Data Universe (OSDU)[®] Data Platform is a data ecosystem for the energy industry, with the aim to standardise data formats so that reservoir characterisation and production data can be shared, integrated and analysed. The Platform is cloud native and AI ready. The Open Footprint[®] Data Model maps and transform technical data to emissions activities, specified carbon accounting methodologies and reporting boundaries. The two forums liaised two years ago to establish a CCUS harmonisation project to manage and monitor subsurface and carbon footprint data. OSDU's Production Data Management (PDM) uses a detailed technical model for CCUS process data and monitoring systems, including flow modelling, product volume summaries and downtime event management. Data ingestion and consumption is one of the main problems today with regards of using AI models in this area, i.e. real-time data can sometimes come in in microsecond intervals, so storing this data in a consistent format and making it available to stakeholders is essential, especially when it comes to monetisation.

Generative AI can assist the CCUS virtual supply chain by identifying data mapping and ingestion pathways for structured and unstructured data sources. Retrieval Augmented Generation (RAG) processes can be used to identify and extract patterns in source data to automate data workflows. Further, AI can help connecting source data to transformers for real-time processing and reporting. Finally, it can assist in the development of strategies to track and verify the quality of recorded data and reconcile discrepancies.

Jon then handed over to Bertrand, who talked about how to integrate disparate sources and legacy systems into the CCUS supply chain with the help of AI enabled data ingestion workflows. Here, generative AI is used to automate the data sourcing, mapping, ingestion and validation. One of the main aims is to ensure data traceability and accuracy, ultimately enabling a System of Record (SOR) and the establishment of digital twins.

Session 8: AI-Powered Activity-Based GHG Emission Calculation

Jerome Mutschler (Demetrix) gave a brief overview of the tool that Demetrix has developed to help companies better estimate their Scope 3 greenhouse gas (GHG) emissions by automating the lifecycle assessment (LCA) of a company's purchased products.

Quantifying GHG emissions using the activity-based method is currently challenging, due to the involved complexity (thousands of purchased products, i.e. data points), low quality (i.e. incomplete) data and associated high costs. AI can help to improve this process by making it simpler through the automated calculation of Scope 3 emissions with proprietary algorithms, increase data accuracy through enhanced data integration and enrichment, and reduce the costs through streamlined workflows and error reduction. The product GHG footprint of the products is reverse engineered through a product material breakdown and drawing from LCI (life cycle inventory) databases. The tool can extract unstructured data, such as from client bills and then allows an estimation of the related CO₂e emissions.

The goal is to perform AI-driven LCAs to help companies, including those operating in the CCUS sector, to determine whether their system captures more CO₂ than is emitted.

Interactive Breakout Groups

Opening Remarks

This collaborative real-time exercise in Breakout Groups focused on exploring how AI can support and accelerate safe and effective CO₂ deployment during all stages of the CCUS chain, i.e. capture, transport and storage, and across the supply chain. Participants from diverse technical and organisational backgrounds worked together across structured e-whiteboard workspaces to examine key challenges, assess current capabilities, identify roadblocks and risks, and propose actionable mitigation solutions. This interactive format enabled a rich exchange of insights on the role of AI throughout the CCUS chain.

Breakout 1: AI in CO₂ Capture

Thematic Focus 1: Most Pressing Questions

The participants of the breakout group identified many pressing questions that currently exist when considering the use of AI in CO₂ capture. This included on a general level how AI can accelerate the selection and optimization of CO₂ capture technologies in different industrial contexts, how to ensure interpretability and reliability of AI models in capture

process optimization, and what datasets and standards are needed to train trustworthy AI models for CCUS.

In detail, participants questioned how to apply AI to the operation of a capture plant, e.g. operational decisions as the plant experiences new operational challenges, and the synchronisation of the capture plant with the point source during the start-up phase. Here, AI could be used to optimise several different areas, such as process/reactor design, solvent selection/material discovery, reduction of capital cost, operating cost, and energy consumption, and maximising profits via monitoring electricity prices. Similar to the work presented on Day 1 of the workshop on MOFS, absorption solvents need to be screened for low reboiler duty, high absorption capacity, rapid kinetics, low degradation, low corrosion based on mass transfer, chemical kinetics, thermodynamic equilibrium etc. Packing wetting/channelling is a critical issue during changing operational conditions (off design operation), and AI-assisted tomography technology to monitor the packing and tune the operation to avoid such a situation could be useful. For using AI in the optimisation of the operation of the capture plant, reliably monitoring CO₂ purity, flow rate, and capture efficiency in real time will be essential.

One related question was how AI can help in flexible operation of CO₂ capture plants. This includes flexibility to respond to load changes of the parent plant due to intermittent renewables and variations of CO₂ concentration and flue gas flow (e.g. by varying solvent flow, stripper conditions, lean loading). AI might also be tasked to optimize the physical footprint of the capture plant.

Another area that was mentioned was using AI to develop a better understanding of the links and risks between flue gas characteristics or composition and degradation of the capture medium, especially amine-based ones, and also to test methods to mitigate this degradation. For this, AI would need to understand the underlying chemistries of solvent degradation. Solvent degradation is a complex phenomenon and needs monitoring, prediction of accelerated degradation based on solvent chemistry and plant operation in real time. AI might also be used to design and optimise the solvent reclaiming process (i.e. when to reclaim and to what extent, avoidance of wasting useful solvent, best technique for solvent management etc.), while at the same time keeping in mind that some species are useful to be in the solvent as they act as degradation inhibitors. Emissions from carbon capture plants, some of which are carcinogenic (i.e. nitrosamines and nitramines from amine solvents), were mentioned as a growing concern. These emissions, including other solvent components and substances formed within the capture system, can have environmental impacts and require careful assessment, permitting and monitoring to avoid negatively affecting public health and perception.

Finally, participants questioned how the conflict of human vs AI opinion, especially with a maturing AI, can be resolved, and how AI models developed for CO₂ capture can be integrated with overall CCUS value chain assessments (which might be using AI as well).

Thematic Focus 2: State of the Art and Mature Solutions

This session discussed both current and emerging applications of AI/ML in CO₂ capture. Participants highlighted other early-stage solutions, which included: surrogate models of physics-based simulators (e.g., Aspen, gPROMS) for rapid screening, AI models predicting solvent performance (e.g., absorption capacity, regeneration energy consumption) using molecular descriptors, general process optimisation and predictive control, and tools developed for accelerated material discovery. The use of digital twins with integrated AI for monitoring and optimizing post-combustion capture units, including predicting failures, making informed decisions with real-time data for simulation, testing, monitoring, and analysis, were mentioned as mature solutions. Hybrid approaches, such as high-fidelity models in combination with AI models, are being researched as well.

Thematic Focus 3: Roadblocks and Risks

In a next step, the participants of the breakout group identified several risk and roadblock of using AI in CO₂ capture. One significant concern is the high computational cost for coupling AI with detailed process simulators or CFD models. This is also directly related to GHG emissions from powering the required data centres, and the question to what extent these can be supplied with low-carbon/clean energy. In addition, the implementation of AI requires investment for development and validation. If the roll-out of data centre and supercomputer infrastructure does not happen quickly, this could be a bottleneck for wider use of AI in CO₂ capture.

Another area that was highlighted both in this session and during the workshop presentations on Day 1 were trust and reliability. A lack of trust or understanding of risks with AI could potentially negatively affect the public perception and social-license-to-operate of AI technology. There could be resistance to adopting black-box AI models, especially in safety-critical industrial settings. Knowing the capabilities of AI and associated risks will be crucial to understand and minimise uncertainty in AI techniques and model bias.

Participants also agreed that data availability at large scale to train AI models could pose a risk. Concerns of technology developers with sharing of their proprietary process knowledge feeds into this, but also information sharing across CCUS and AI experts was seen as challenge. Both could contribute to the formations of research silos (both CCUS and AI related). Other aspects that were mentioned during the discussion included limited high-quality, diverse datasets for training robust AI models, and the lack of standardized protocols for AI model validation.

Thematic Focus 4: Mitigation

The final round of discussion focused on potential mitigation strategies. Participants mentioned that the limited availability of high-quality datasets could be overcome by fostering industry-academia-government data sharing frameworks, using synthetic data from high-fidelity simulators and applying transfer learning and data augmentation. Developing benchmarking datasets and evaluation protocols for capture technologies could help alleviate the current lack of standardized protocols for AI model validation.

Against the high computational cost of integrated AI/simulation models, development of efficient surrogate models (e.g. neural nets trained on simulator outputs) and the use of high-performance/cloud/quantum computing resources with parallel pipelines could help. Also, finding the best available AI technique or combination of techniques for a particular application will be helpful.

In order to improve the low trust in black-box AI models, the promotion of causality analysis and interpretable ML (e.g. model-agnostic XAI methods such as SHAP (SHapley Additive exPlanations), LIME (Local Interpretable Model-agnostic Explanations)), plus the involvement of domain experts in model development and validation are promising mitigation options. Networking, collaboration and capacity building between CCUS and AI experts will be essential to share knowledge and to create awareness about AI pros and cons to trust the AI application in CCUS with respect to IP issues and to build trust with community stakeholders.

To improve generalisability of AI models to mitigate inherent potential biases it will be necessary to increase AI/ML competencies, i.e. a focussed training of existing and next generation CCUS and AI experts. In addition, AI models need to be tested at scale, which will require an increase of funding for AI development based on partnership between industries and research centres/universities.

BO – 1 Concluding Remarks

AI holds significant promise for enhancing CO₂ capture technologies, particularly in optimizing operations, reducing costs, and improving energy efficiency. Its potential spans from material discovery to real-time plant control.

Data availability and sharing remain major bottlenecks. Proprietary concerns and siloed research hinder progress. Collaborative frameworks across industry, academia, and government are needed to unlock high-quality datasets. Training the next generation of CCUS and AI experts, and fostering cross-domain partnerships, will be key to successful AI deployment.

Interpretability and trust in AI models are critical. Black-box models face resistance, especially in safety-critical environments. Transparent, explainable AI approaches and expert involvement are essential to build confidence.

Environmental and health risks, such as emissions from degraded solvents, must be carefully monitored. AI can aid in predicting and mitigating these risks, but this must be aligned with regulatory and public health standards.

Computational demands of AI integration with detailed simulations pose environmental and infrastructure challenges. Efficient models and data centres with low-carbon energy supply can help mitigate these issues.

Breakout 2: AI in CO₂ Transport

Thematic Focus 1: Most Pressing Questions

Participants of this breakout group started identifying the most pressing questions and issues related to the use of AI in CO₂ transport. The first area discussed was the concept of 'CO₂ as a molecule that moves', and how we can use AI when it comes to getting the phase data (i.e. pressure, temperature, quality, and impurities). This includes improving and optimizing the instrumentation to predict the stream characteristics of CO₂. AI could help here with ensuring modelling integrity by integrating upstream data/processes to ensure that the CO₂ streams are within the specifications. This might go as far as modelling digital twins for gas mixtures. AI modelling can also be used for identifying what the best mode of transport is (i.e. pipeline, ship, truck, rail or barge), as well as optimising/predicting how much of the CO₂ should go to permanent geological storage and how much to downstream processing (i.e. utilisation) or enhanced oil recovery (EOR). A further question is how to apply AI in modelling for safety related to leaks, monitoring devices and optimization of the related instrumentation, i.e. ensuring the CO₂ balance across the transport network.

Another part of the discussion focussed on "hardware" aspects. This includes using AI models for: identifying the best as well as new materials of construction factoring in CO₂ characteristics, "merging" or "refactoring" the green field and re-purposed pipelines, optimising the use of non-pipeline transport options, and using digital twin for predictive maintenance.

Participants then moved on to identify issues related to the tracking or movement of CO₂ across the network. This includes how to use AI to tag CO₂ molecules to help ensure sustainability, i.e. carbon intensity of a product or service and for this, AI-assisted MRV (Measurement, Reporting, and Verification) could play a role. Questions remain on how to optimise the transport or "traffic of CO₂" and how to track and trace "nominations". AI could be used in financial simulations and the design of digital twins to aid permitting

and the issuance of carbon credits by regulatory agencies, including using AI to prevent double counting of credits.

Thematic Focus 2: State of the Art and Mature Solutions

Building on the discussion above, participants then started to identify existing and emerging uses of AI in the field of CO₂ transport. The first area mentioned was the use of predictive software for thermodynamic models for CO₂ (both dynamic and static). CFD model as are used for modelling leaks, supply chain modelling software is used for helping decide the mode of transport, and there is software available for a standardized engineering specification (e.g., JIP33 compliance). Models can also determine on the best mode to utilize the transported CO₂ directly at final or intermediate locations

In addition, software for predictive maintenance can optimise the best material of construction (JIP33). Ultimately, "grand" models can emerge that factor in financial modelling and sustainability aspects of the transport, i.e. using AI for MRV (for regulatory, audits, and document management), using digital twins to tag CO₂ and aggregate to a "blockchain" type platform, but also using AI in social media to avert community risks (e.g. predicting the sentiment of society).

Thematic Focus 3: Roadblocks and Risks

During this session, participants discussed potential roadblocks and risks related to the use of AI in CO₂ transport. AI-specific roadblocks that were identified include the energy consumption of AI models as well as general cybersecurity. Many concerns are related to data, i.e. the volumes of data that need to be processed/integrated, data security and proprietary, data standardisation and management, data quality and availability, and interpretability of data for different industries.

With regards to technical risks, participants brought up potential equipment failure, caused or exacerbated by corrosion and degradation, unavailability of sensors and analysers that are of high enough accuracy (leading to low quality input data, and thus GIGO), operational and logistical roadblocks, scaling and safety risks.

Among non-technical risks, financial issues, such as economic viability of both AI model and hardware, as well as availability of insurance and liabilities were mentioned.

Regulatory uncertainty is a further risk, e.g. lack of or imbalances in regulatory frameworks, permitting on certain (e.g. tribal) lands, lack of data sharing standards. Questions remain how to ensure traceability and linkage to environmental, social and governance (ESG) reporting. Finally, there are risks related to social and community acceptance of both AI and CO₂ transport, as well as educational aspects.

Thematic Focus 4: Mitigation

Participants identified several mitigation approaches for the AI-specific roadblocks discussed in the previous section. Advanced circuitry that reduces energy consumption and optimised algorithms that reduce processing power were highlighted. In addition, immutable logging, global AI safety frameworks and regional, national, and global standardisation frameworks are necessary. Compliance tools could help with automatically tracking regulatory changes and interpret those regulatory frameworks to capture the changes and future proof the data domain. Besides, dynamic compliance tools can help understand the limitations of certain standards when it comes to feeding them into AI tools.

Mitigation options for the technical and non-technical risks include the expansion of experimental data to enrich the digital twins/AI models. R&D on advanced sensors will be required, not only to improve efficiency, quality, and accuracy, but also to decrease cost so we can deploy more. Improvement of general compliance and adherence to frameworks in risk management was also mentioned. In addition, participants highlighted the development and use of educational AI tools that are aimed at identifying what works best for society factoring in different demographics and interests.

Supplementary Notes

Participants highlighted additional topics that they felt were of high interest when discussing the use of AI in CO₂ transport. Among them was, e.g., the use of satellite technology to monitor CO₂ pipelines leaks and feed this data into AI models. It was mentioned that the same technology platforms that we use for CH₄ can also be extended to CO₂. Blockchain was mentioned as an interesting concept, with some participants being particularly interested in seeing how digital twins can be married with blockchain. Digital assets and/or tokenisation of the CO₂ could make it tradable “straight from the sensors”. Further issues that were highlighted included the general education on the importance of AI for CO₂ transport and the importance of Article 6 and the translation to national laws in the context of AI use in carbon management chains.

BO – 2 Concluding Remarks

AI has transformative potential in optimizing CO₂ transport systems—from modelling physical properties and selecting transport modes to ensuring safe and sustainable operation.

Digital twins and predictive models are central to improving operational efficiency, enabling real-time monitoring, and supporting decision-making across the CO₂ value chain.

Key risks include high energy consumption of AI models, cybersecurity threats, data quality and standardisation issues, and societal acceptance of both AI and CO₂ transport infrastructure.

Thus, mitigation strategies must focus on developing energy-efficient AI hardware and algorithms, as well as global and regional standards for data compliance. Promoting education and public engagement to build trust and understanding will be essential, too.

Policy alignment, especially with frameworks like Article 6 of the Paris Agreement, is essential to ensure AI applications in CO₂ transport are legally grounded. AI-assisted MRV can enhance traceability, support regulatory compliance, and prevent issues like double counting in carbon credit systems. In addition, emerging technologies like satellite monitoring and blockchain integration offer promising avenues for enhancing transparency, traceability, and tradability of CO₂.

Breakout 3: AI in CO₂ Storage

Thematic Focus 1: Most Pressing Questions

Participants identified several persistent challenges limiting the effective use of AI in CO₂ storage. These included permitting bottlenecks, regulatory delays, and gaps in tracking project obligations. Concerns around trust and reliability featured prominently, particularly in relation to the opacity of 'black-box' models and the risk of false or misleading outputs. The lack of shared, standardised datasets especially for training AI in anomaly and leak detection was highlighted as a key technical barrier, along with questions about cross-site model transferability and platform compatibility. Additional challenges included high costs associated with injection materials and the optimisation of surface processes. In the MMV and subsurface domains, participants emphasised the need for improved AI tools to support conformance analysis, integrity assessment, uncertainty quantification, and history matching.

Thematic Focus 2: State of the Art and Mature Solutions

This session highlighted both current and emerging applications of AI in CO₂ storage. Participants discussed the use of U-Nets and physics-informed neural networks (PINNs) for subsurface interpretation. Digital twin platforms were recognised for their role in enhancing real-time monitoring and operational efficiency. While automated anomaly detection in pressure and microseismic data is gaining traction, it was noted as an area still under development. Proxy simulators integrated with conventional modelling tools are helping to accelerate workflows, though there remains a gap in the availability of robust AI-driven model generators. On the regulatory front, innovations such as large language models (LLMs) and AI-enabled tools to support Class VI permit preparation were seen as promising. Collectively, these developments reflect the emerging role of AI deployment in CO₂ storage, while also underscoring the need to close remaining capability gaps.

Thematic Focus 3: Roadblocks and Risks

Participants identified several critical risks that could impede AI integration in CO₂ storage. Regulatory and stakeholder acceptance emerged as foundational concerns, underscoring the importance of explainability and trust in AI systems. The limited transferability of models across different geological settings was highlighted as a barrier to generalisability. It was broadly agreed that AI tools should augment but not replace expert judgement, particularly in complex geoscience contexts.

Key technical constraints included limited computational resources, a shortage of AI-skilled personnel, and uncertainty around the industry's readiness to invest in large-scale model development. Broader systemic concerns were also raised, such as the absence of a sustainable business model for AI deployment across the CCS chain.

Data-related issues were especially prominent, ranging from poor data fidelity to the lack of standardised benchmarks and frameworks for evaluating AI solutions. Inadequate or biased training datasets, along with risks such as overfitting and the omission of edge cases, were flagged as significant obstacles. Participants also cautioned against overreliance on AI, often driven by hype or misplaced confidence in model outputs. Finally, intellectual property barriers and persistent data silos continue to limit collaboration and hinder the development of shared tools and resources.

Thematic Focus 4: Mitigation

The final workspace focused on potential mitigation strategies. Participants recommended the establishment of AI quality control (QC) standards and benchmarking protocols aligned with validated traditional methods. Collaborative efforts to develop and share benchmarking datasets were seen as a priority to promote transparency, comparability, and trust.

Robust validation approaches such as cross-validation, adversarial testing, and explainable AI (XAI) were proposed to enhance interpretability and support regulatory acceptance. Broader education and training initiatives were viewed as essential, not only for technical teams but also for regulators and stakeholders, to foster AI literacy and enable early engagement. Case studies were encouraged as practical tools to build confidence and demonstrate real-world value.

Data sharing, particularly for MMV, was proposed as a permitting requirement in CCS hubs. In addition, participants highlighted the need for clearer frameworks governing model ownership and intellectual property (IP) rights in co-development scenarios, to incentivise collaboration while protecting innovation.

BO – 3 Concluding Remarks

A consistent theme throughout the breakout session was the transformative potential of AI to enhance subsurface workflows, risk analysis, monitoring, and permitting. However,

participants remained clear-eyed about the significant challenges particularly around data quality, trust, regulatory acceptance, and resourcing that must be addressed to fully unlock this potential.

To enable scalable, long-term deployment of AI in CCS, the group emphasised the need for interdisciplinary training, stronger data standards, proactive regulatory engagement, and transparent validation frameworks. Ultimately, the success of AI in CO₂ storage will depend not only on technical innovation, but also on building trust through explainable, collaborative, and context-aware solutions that reflect the needs of the broader CCS value chain.

Breakout 4: AI in CO₂ Supply Chains

Thematic Focus 1: Most Pressing Questions

A central concern was regulatory compliance, particularly with regard to measurement, monitoring, and verification (MMV) processes, and the potential role of AI in accelerating permitting and streamlining regulatory checklists across jurisdictions. The group emphasised the need to make CCS regulations and reporting more AI-compatible, and to embed automation into regulatory and reporting workflows.

Another prominent theme was the lack of digital integration across the supply chain from capture through transport to storage. Participants highlighted the importance of digitising and linking system components to enable seamless data flow and strengthen AI-supported decision-making. AI's role in risk management, carbon credit verification, and transparent certification also featured strongly in the discussion.

Additional technical and operational challenges included the development of intuitive, interoperable systems, tools for self-navigation and automation, and education initiatives aimed at harmonising language and understanding across different parts of the value chain.

Thematic Focus 2: State of the Art Solutions (Early-Stage and Mature)

Building on these challenges, participants explored existing and emerging solutions currently being applied or piloted. Tools such as Baker Hughes' CarbonEdge an end-to-end solution for CCUS operations and CarbonSolutions LLC, referenced in the context of strategic planning, were noted for their potential impact.

Participants also highlighted ongoing efforts to integrate modelling with real-time operations and the development of AI-assisted tools for regulatory compliance. These

examples suggest that foundational AI-enabled capabilities are beginning to mature and gain traction within the CO₂ supply chain.

Thematic Focus 3: Potential Roadblocks and Risks

Despite emerging solutions, participants highlighted several persistent roadblocks. A major concern was the inaccessibility or unavailability of key data, compounded by biases in existing datasets, which limit the ability to train robust and generalisable AI models.

Challenges related to data sharing and integration were also discussed. In particular, confidentiality concerns and operational silos especially between emitters and transport or storage operators were seen as significant barriers to cross-chain optimisation.

Participants also expressed concern that many stakeholders remain in the early phases of project development and are therefore not yet considering how AI could be incorporated. This lack of forward planning may delay or limit future AI deployment.

In addition, explainability and trust emerged as critical themes. Concerns were raised about “black-box” decision-making, particularly in light of emerging policy frameworks such as the EU AI Act, which may require greater transparency and accountability in AI systems.

Thematic Focus 4: Potential Mitigation vs Roadblocks

To address these challenges, participants proposed a range of mitigation strategies. A key recommendation was to embed explainability at the AI model development phase, rather than treating it as a post hoc requirement. The use of case studies and small-scale pilot projects was encouraged to demonstrate AI's value and build confidence among users and regulators.

Improving data structure and quality was also emphasised, with participants advocating for tools to convert unstructured data into structured formats to facilitate integration and analysis. Standardisation across the supply chain including the development of anonymised, decentralised data-sharing systems was seen as critical to overcoming resistance to collaboration.

Supplementary Notes

Additional discussion highlighted the dynamic nature of regulatory environments and the need for adaptable AI systems that can respond to changing rules and expectations. The

development of decentralised reporting mechanisms that maintain data anonymity without compromising traceability was recommended.

Participants reiterated the importance of consistency in MMV compliance across jurisdictions and stressed that data harmonisation should remain a central goal.

BO - 4 Closing Remarks

The discussions in Breakout 4 reaffirmed the significant potential for AI to enhance efficiency, transparency, and decision making across the CO₂ supply chain. However, realising this potential will depend on the sector's ability to address pressing challenges related to data quality, integration, regulatory alignment, and stakeholder trust.

Participants underscored that forward-thinking investment in infrastructure, cross-sector collaboration, and adaptive regulatory frameworks will be essential to enable AI to scale effectively. Education, transparency, and early demonstration of value will play a vital role in building the confidence needed for broader adoption.

In conclusion, the breakout session called for a coordinated, inclusive approach to AI deployment, one that ensures innovations are not only technically advanced, but also explainable, interoperable, and responsive to the practical needs of CO₂ supply chain actors.

Conclusions and recommendations

Conclusions

AI is a transformative enabler for CCUS. Across the CCUS value chain—from capture and transport to storage and supply chain management—AI has demonstrated significant potential to accelerate innovation, improve operational efficiency, and reduce costs.

Real-world applications are emerging. Case studies from industry and academic leaders show that AI is already being used to enhance material discovery, automate subsurface analysis, streamline permitting, and monitor CO₂ transport and storage.

Trust, transparency, and explainability are critical. The adoption of AI in safety-critical and regulatory contexts requires models that are interpretable and auditable. Black-box systems face resistance, especially in permitting and public engagement.

Data remains a major bottleneck. High-quality, diverse, and standardised datasets are essential for training robust AI models. Proprietary concerns, siloed research, and lack of

interoperability hinder progress. Lack of high-quality data will likely lead to increased hallucinations/GIGO (garbage in, garbage out).

AI should augment—not replace—human expertise. Across all sessions, speakers and participants agreed that AI must support expert decision-making rather than automate it entirely. Human oversight is essential, especially in risk assessment and regulatory compliance.

Environmental and ethical considerations must be addressed. The energy intensity of AI models, potential biases, and risks of overreliance were highlighted as concerns. Responsible AI development must include sustainability and ethical safeguards.

Recommendations

Establish cross-sector data sharing frameworks. Promote collaboration between industry, academia, and government to unlock proprietary and siloed data, and develop anonymised, decentralised systems for secure data exchange.

Invest in explainable and interpretable AI. Prioritise model transparency from the development phase, and use techniques like SHAP, LIME, and neuro-symbolic AI to improve trust and regulatory acceptance.

Develop benchmarking and validation protocols. Create standardised datasets and evaluation frameworks for AI models in CCUS, and align AI validation with traditional engineering and scientific methods.

Support interdisciplinary training and capacity building. Train CCUS professionals in AI and vice versa and foster communities of practice to bridge gaps between technical domains.

Accelerate permitting with AI tools. Use AI to streamline regulatory workflows, reduce review times and associated costs, and improve completeness checks. Ensure AI tools are designed to capture tacit regulatory knowledge and support human judgement.

Promote energy-efficient AI development. Invest in low-power models (e.g. SLMs) and clean energy-powered data centres. Consider the carbon footprint of AI infrastructure in CCUS planning.

Embed AI into digital twins and MRV systems. Use AI to enhance real-time monitoring and predictive maintenance. Integrate AI into MRV frameworks and blockchain to support carbon credit verification and traceability.

Align AI deployment with evolving policy frameworks. Ensure AI systems comply with emerging regulations (e.g. EU AI Act, Article 6 of the Paris Agreement) and develop adaptive compliance tools to track and interpret regulatory changes.

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