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SimCCS: development and Applications

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Earth and Environmental Sciences

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Development & Applications

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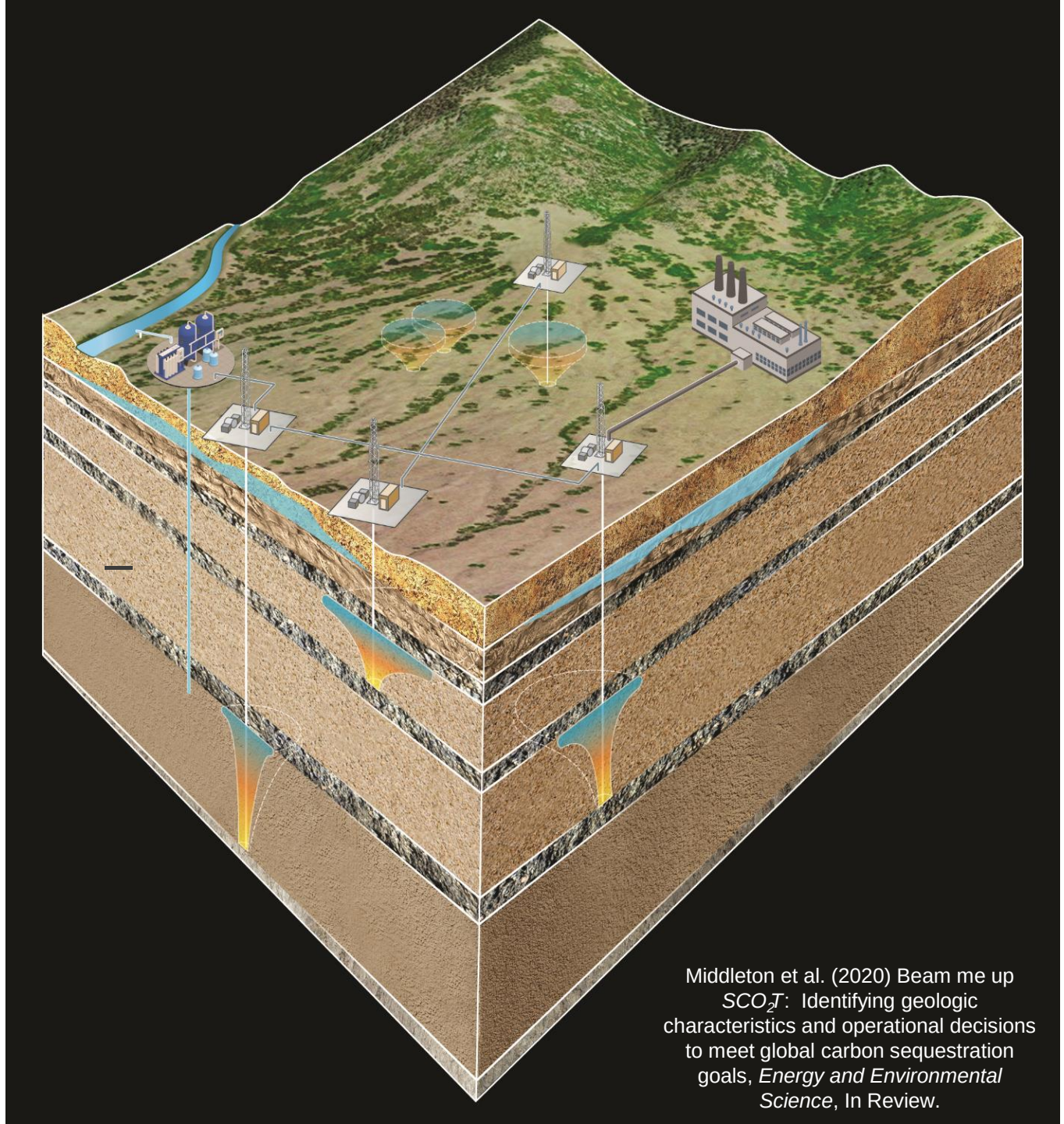
Motivation: Advance the *SimCCS* toolset and further its application.

1: Development

- Fundamental data, tool, & science development.
- Accelerate *SimCCS* integration into DOE-FE projects (e.g., Regional Initiatives, CarbonSAFEs).

2: Applications

- Work with DOE-related initiatives (e.g., National Petroleum Council CCUS report, Regional Carbon Capture Deployment Initiative).
- Collaborate with non-traditional partners such as non-profit institutions.
- Expose DOE projects to *SimCCS* capabilities (e.g., Wyoming CarbonSAFE).

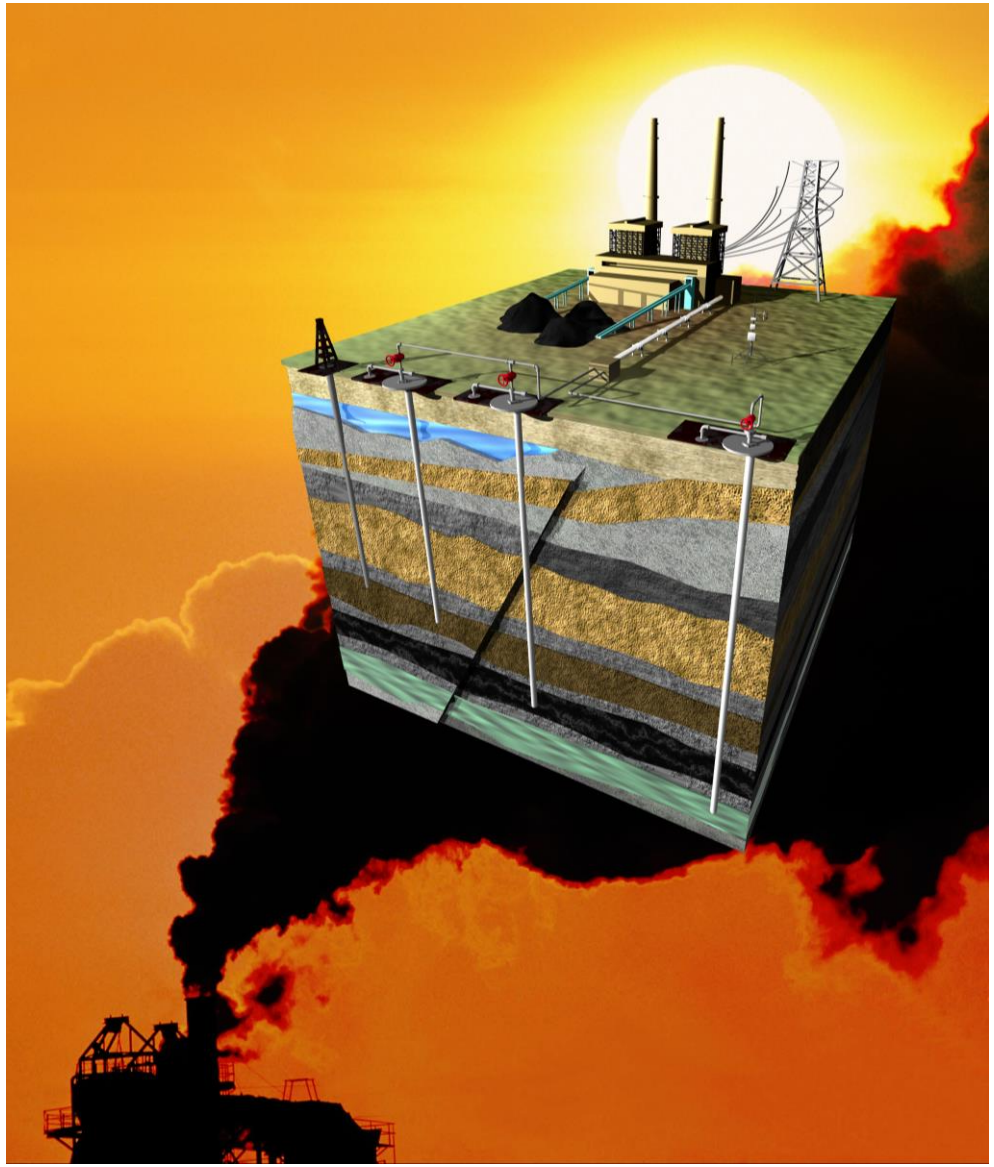


Middleton et al. (2020) Beam me up SCO_2T: Identifying geologic characteristics and operational decisions to meet global carbon sequestration goals, *Energy and Environmental Science*, In Review.

SimCCS: Project History

Projects

1. CO_2-PENS (2009–2011) | Sponsor: DOE | PI: Pawar (LANL).
2. Western Energy Corridor Initiative (2009–10) | Sponsor: DOE | PI: Wolfsberg (LANL).
3. Southern Company case study (2011) | Sponsor: Southern Company | PI: Los Alamos (Middleton)
4. US-China CERC-ACTC (2011–present) | Sponsor: DOE | PI: West Virginia University (Wood).
5. Southwest Regional Partnership on Carbon Sequestration (2016–present) | Sponsor: DOE | PI: University of Utah (McPherson).
6. CarbonSAFEs (2017–present):
   - A. CAB-CS: Central Appalachian Basin CarbonSAFE Integrated Pre-Feasibility Project | Sponsor: DOE | PI: Battelle (Cumming).
   - B. Nebraska Basin CarbonSAFE Integrated Pre-Feasibility Project | Sponsor: DOE | PI: Battelle (Duguid).
   - C. CarbonSAFE in the Northern Michigan Basin Integrated Pre-Feasibility Project | Sponsor: DOE | PI: Battelle (Gupta).
   - D. CarbonSAFE Rocky Mountains Phase I: Ensuring Safe Subsurface Storage of CO_2 in the Intermountain West | Sponsor: DOE | PI: University of Utah (McPherson).
   - E. Establishing an Early CO_2 Storage Complex in Kemper County, Mississippi | Sponsor: DOE | PI: SSEB (Nemeth).
   - F. Integrated Midcontinent Stacked Carbon Storage Hub | Sponsor: DOE | PI: Battelle (Duguid).
   - G. San Juan Basin CarbonSAFE Phase III: Ensuring Safe Subsurface Storage of CO_2 in Saline Reservoirs | Sponsor: DOE | PI: Mexico Institute of Mining and Technology (Balch).
7. *SimCCS*: Development and Applications (2018–Present) | Sponsor: DOE | PI: Los Alamos (Middleton).
8. *SimCCS* heuristic development (2019) | Sponsor: Great Plains Institute | PI: Montana State University (Yaw).
9. Regional Initiative to Accelerate CCUS Deployment (2019–present):
   - A. Regional Initiative to Accelerate CCUS Deployment in the Midwest and Northeastern | Sponsor: DOE | PI: Battelle Memorial Institute (Gupta).
   - B. Carbon Utilization and Storage Partnership (CUSP) of the Western United States | Sponsor: DOE | PI: New Mexico Institute of Mining and Technology (Balch).
   - C. Southeast Regional Carbon Utilization & Storage Partnership (SECARB-USA) | Sponsor: DOE | PI: Southern States Energy Board (Nemeth).



Why, How, What

Why: *Commercial-scale drivers*

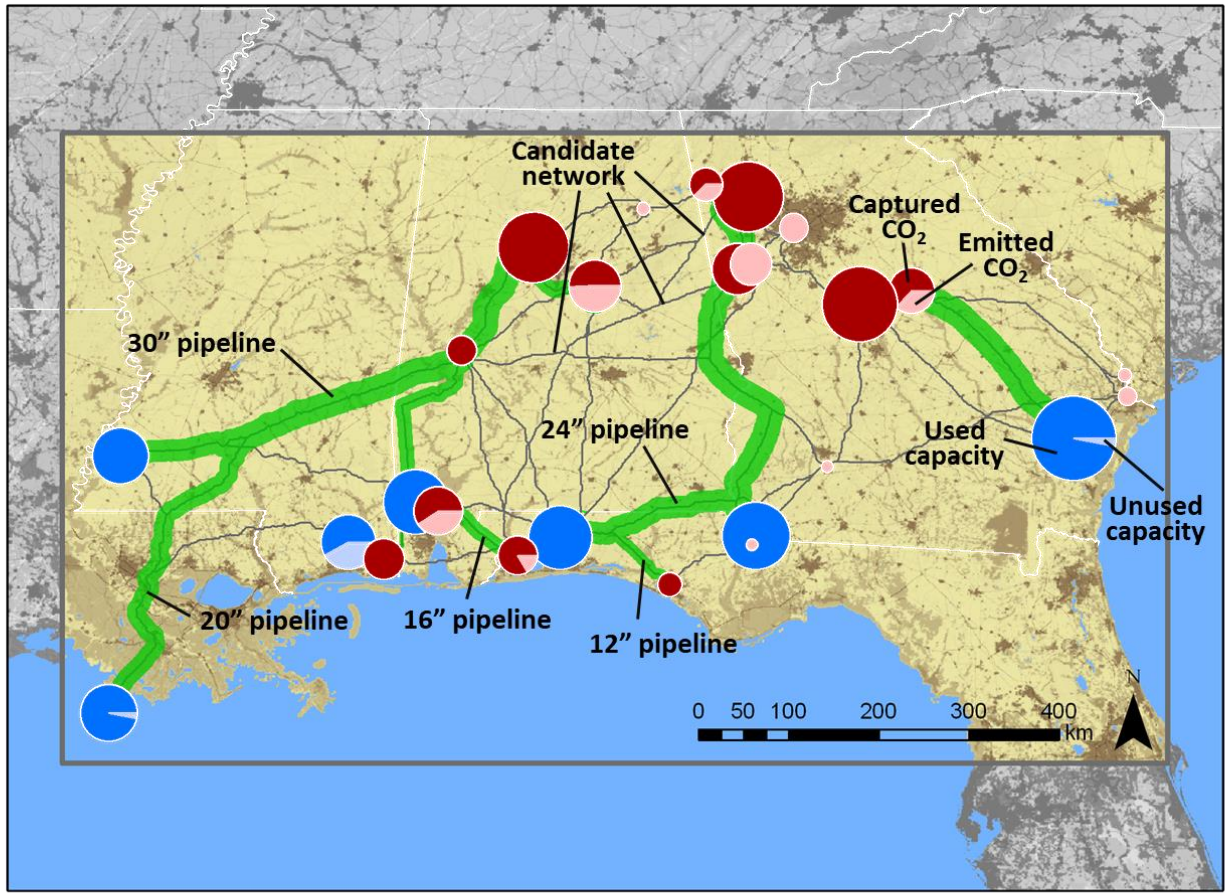
- **GLOBAL**: Climate mitigation policies.
- **US**: Economic incentives (“45Q”).
- **CHINA**: Emissions Trading Scheme (ETS).
- **INDUSTRY**: Carbon footprint reduction.

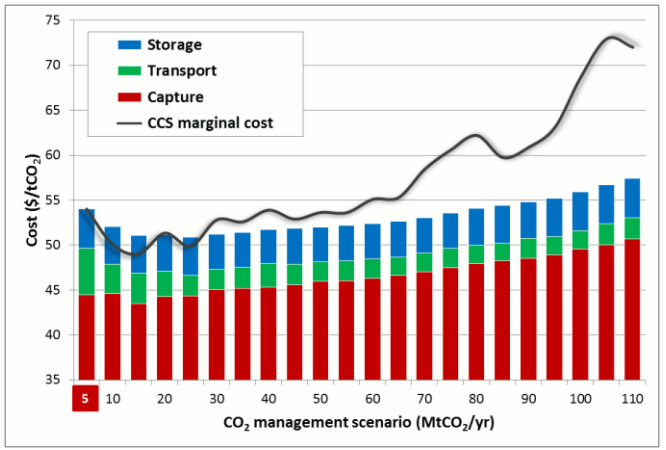
How: *Decision framework for CCS*

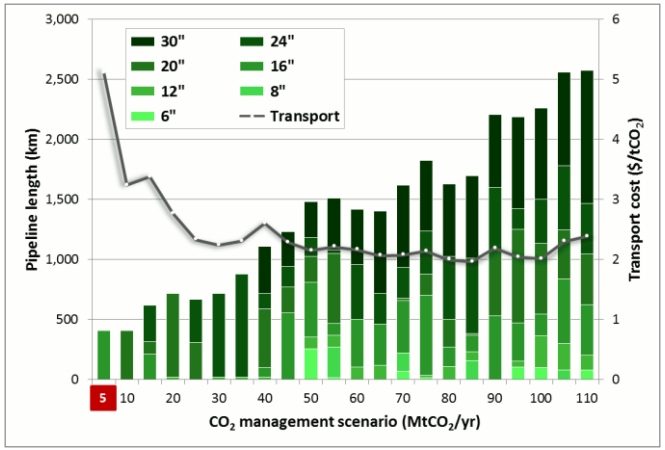
- Design geospatial CCS infrastructure: CO_2 capture, transport, & storage.
- Open-source, Java-based, HPC-enabled framework with desktop & Science Gateway.

What: *Scientific visibility*

- **PAPERS:** 20+ publications, ~1,000 total citations.
- **PEOPLE:** ~100 (published/used/developed).
- **WEBSITE:** *https://simccs.com/*







Middleton *et al.* (2012) The cross-scale science of CO_2 capture and storage: from pore scale to regional scale, *Energy & Environmental Science*

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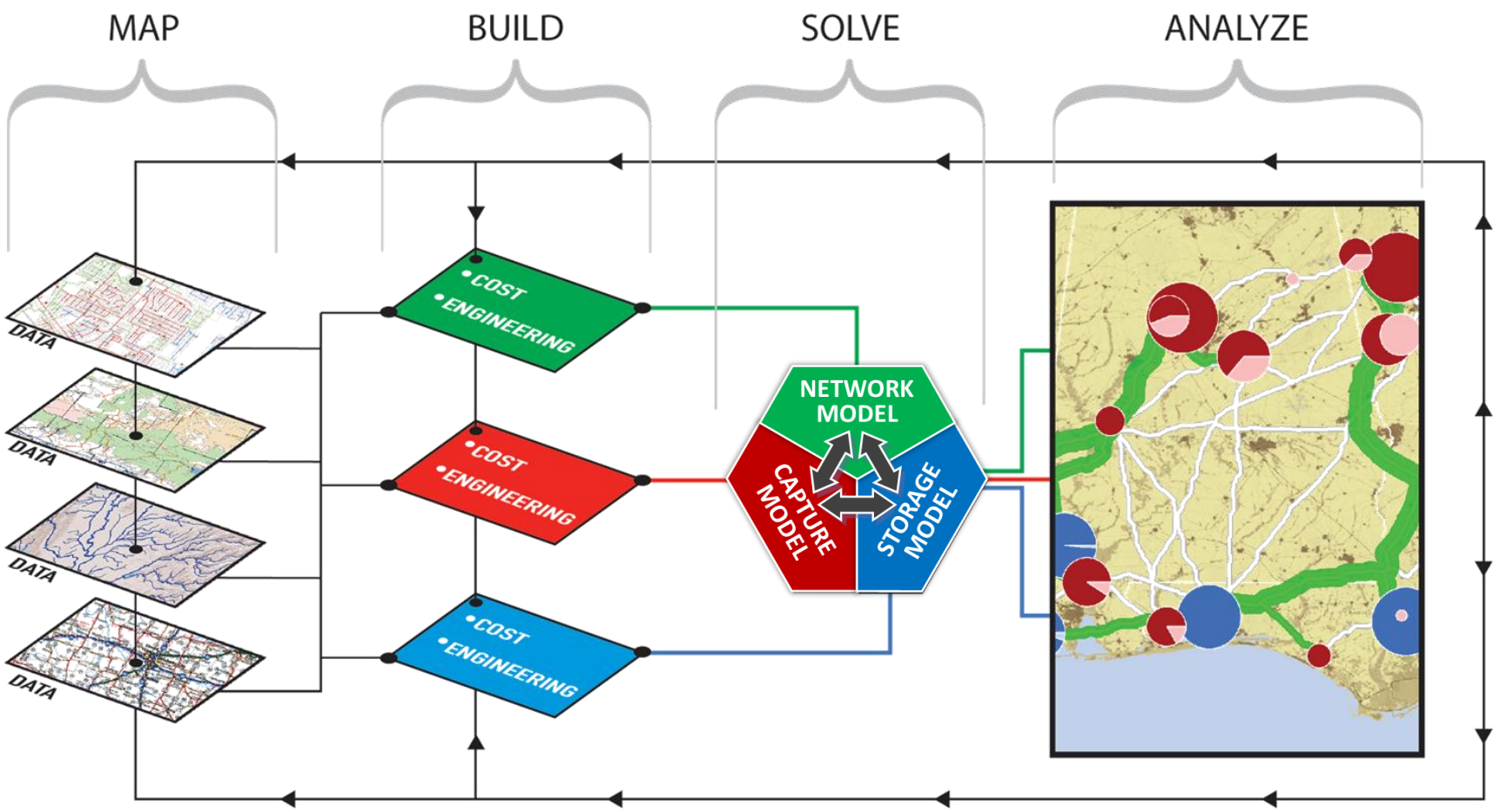
SimCCS Framework
Overview



Middleton *et al.* (2020) *SimCCS*: An open-source tool for optimizing CO_2 capture, transport, and storage, *Environmental Modelling & Software*

Map:

- Unformatted data sources for capture, transport, & storage.

Build:

- Capture, transport, & storage models to build *SimCCS* input data.

Solve:

- **Core:** Linear program
- **Optimization engine:** HPC, desktop solver, or heuristic.

Analyze:

- Export & analyze *SimCCS* data.

SimCCS Interfaces:

- *https://simccs.com/*
- Desktop version.
- Science Gateway version.

BUILD: CAPTURE

NICO$_2$LE

Why?

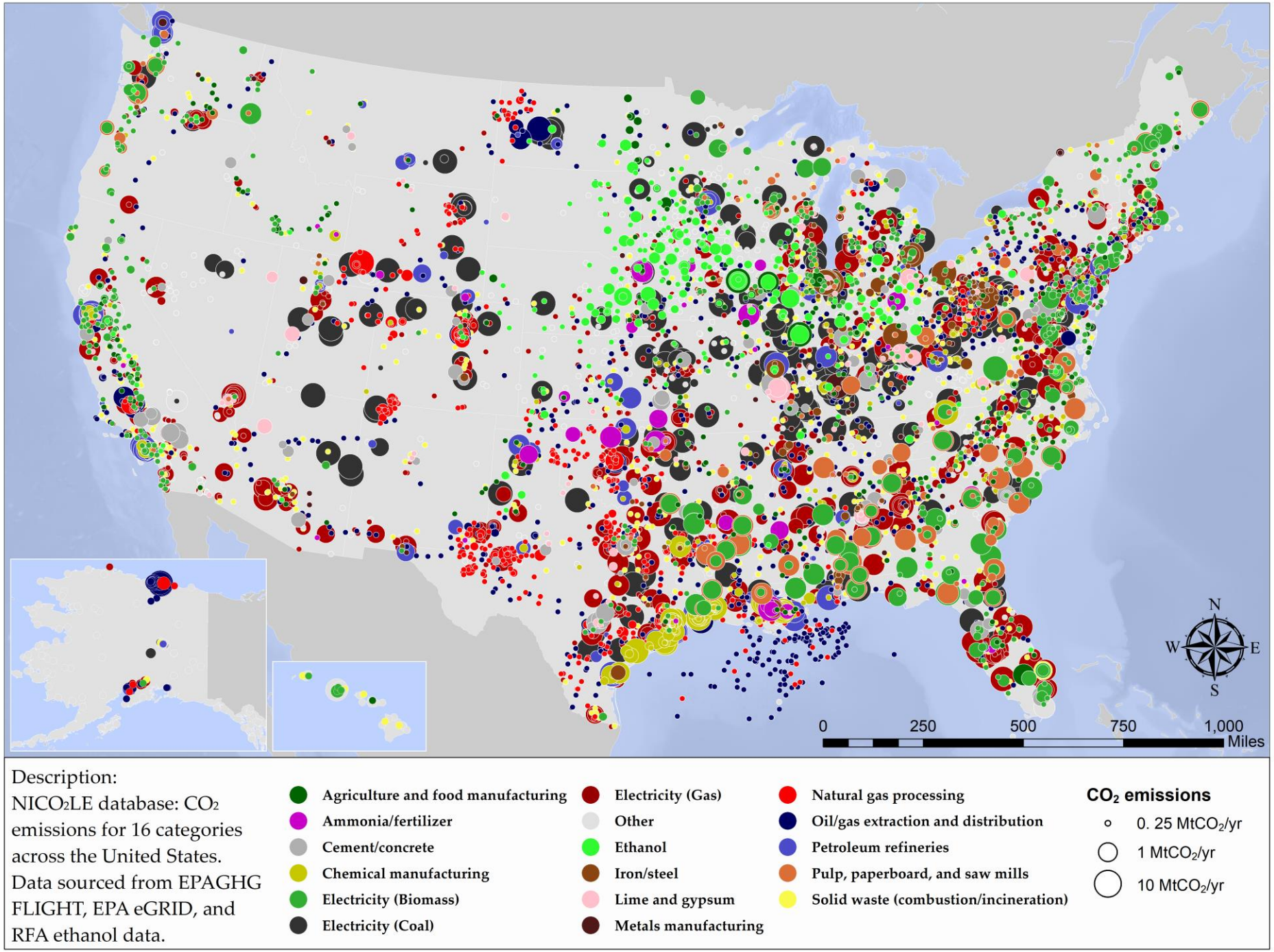
- Identify commercial-scale CO_2 capture opportunities.

How?

- **FUSE:** data from EPA GHGRP/FLIGHT, EPA eGRID, RFA (ethanol)…
- **Fuse:** data from 15+ literature sources for CO_2 streams & capture costs.

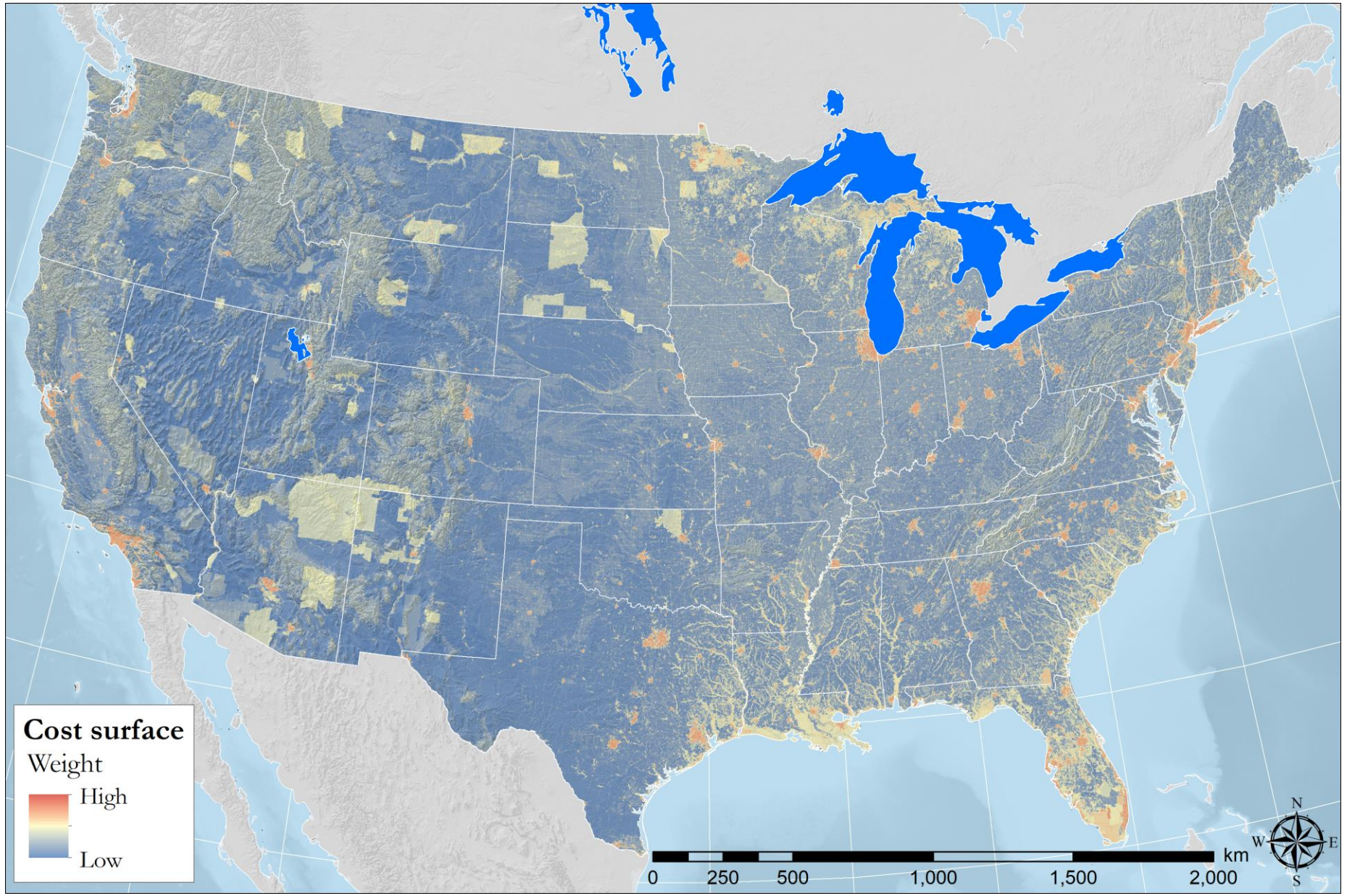
What?

- **GEODATABASE:** source locations, CO_2 streams, & capture costs.
- **SUPPLY CURVES:** Identify economic opportunities.



Middleton *et al.* (2017) Industrial CO_2 and carbon capture: near-term benefit, long-term necessity, *Energy Procedia*

CostMAP



Why?

- **NECESSITY:** Where, how, & cost of CO_2 pipelines.

How?

- Nonlinear integration of ROWs (e.g., pipelines), barriers (e.g., rivers), population, topography, land use, ownership…
- *SimCCS* cost model.

What?

- New approach & software for developing cost & routing surfaces.
- Cost & routing surfaces, grid cells 100–1,000 m.

Yaw *et al.* (2019) Graph Simplification for Infrastructure Network Design, *International Conference on Combinatorial Optimization and Applications*

Hoover *et al.* (2020) *CostMAP*: an open-source software package for developing cost surfaces using a multi-scale search kernel, *IJGIS*

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BUILD: STORAGE

SCO_2T

Why?

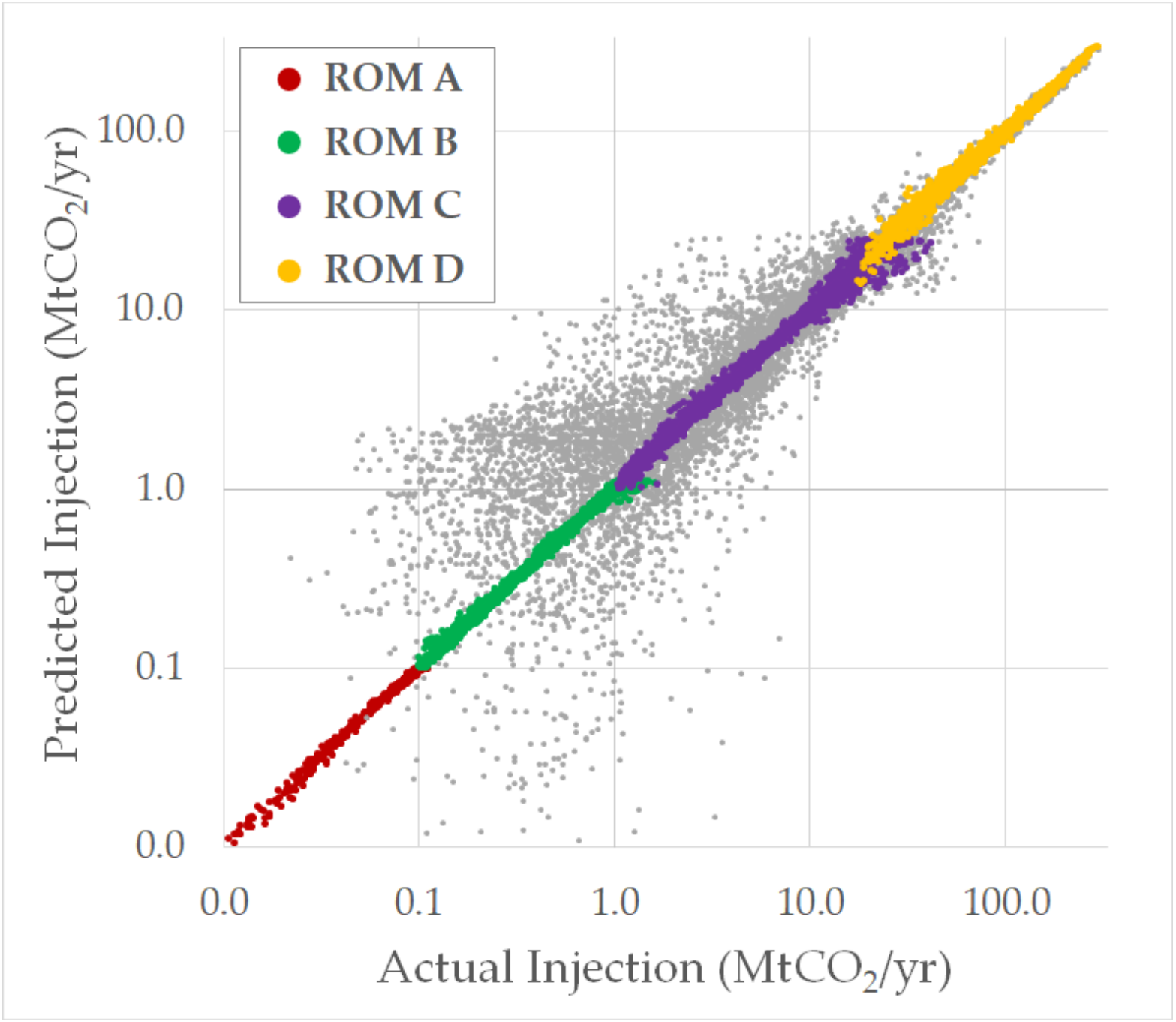
- Rapidly calculate realistic injection & storage & costs.

How?

- Build reduced-order models (ROMs) for CO_2 injection & plume dynamics.
- New ROMster approach for fusing ROMs.
- Connect dynamic CO_2 injection & storage with economics.

What?

- Excel-based tool for rapidly (1000s of realizations per second) calculating dynamic CO_2 injection, storage & costs.



Chen at al. (2019) Frankenstein's ROMster: Potential Pitfalls of Reduced-Order Model Development in CO_2 Sequestration, *IJGGC*

BUILD: STORAGE

SCO_2T

Sensitivity analysis

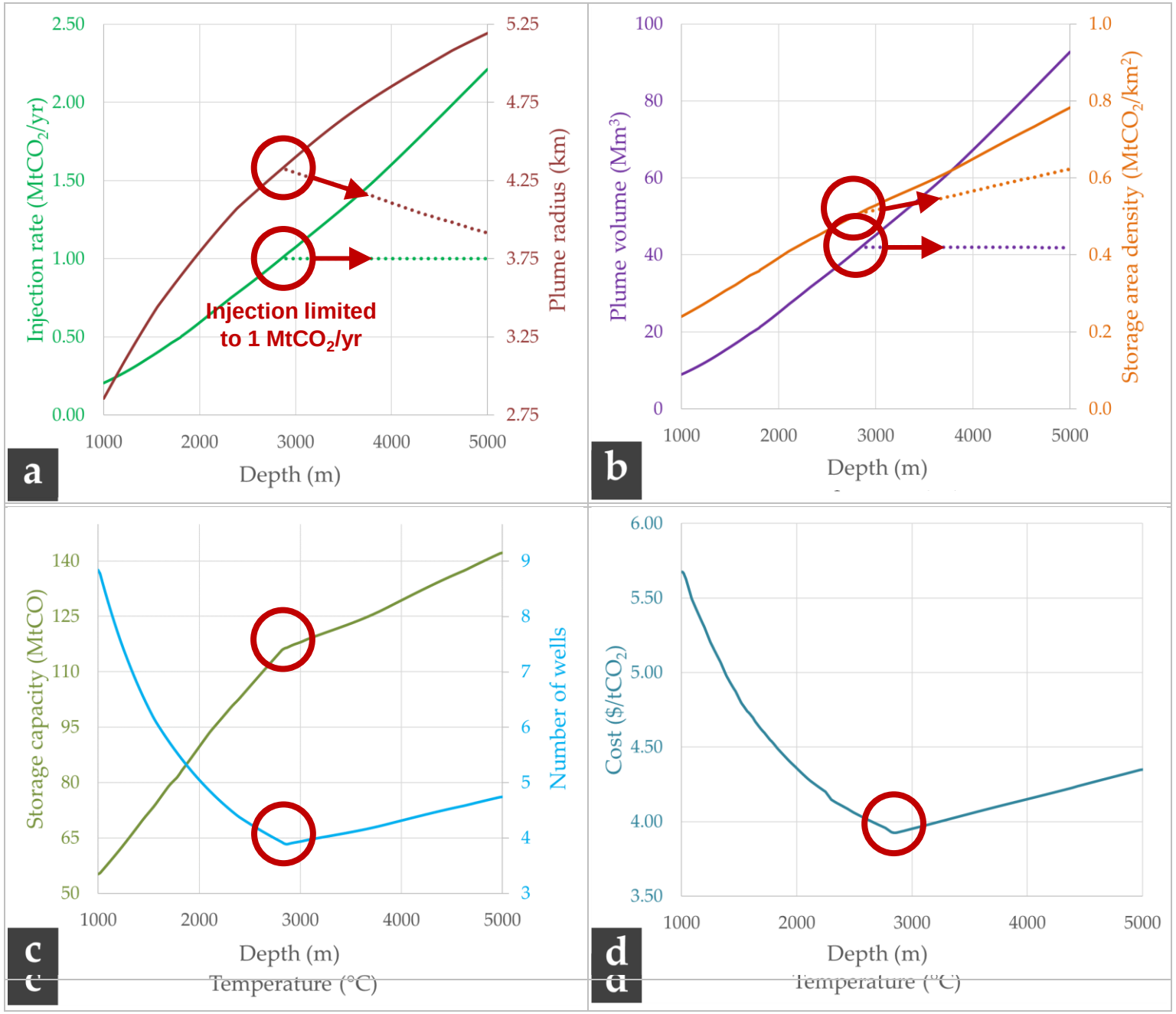
- Identify geologic parameters & combinations that have the greatest impact.

Uncertainty analysis

- Quantify impact of uncertain geologic characteristics including injection rates & costs.

Sequestration science

- Impact of limiting injection rates to 1 $MtCO_2$/yr.
- Impact of increasing depth.
- Impact of brine treatment.



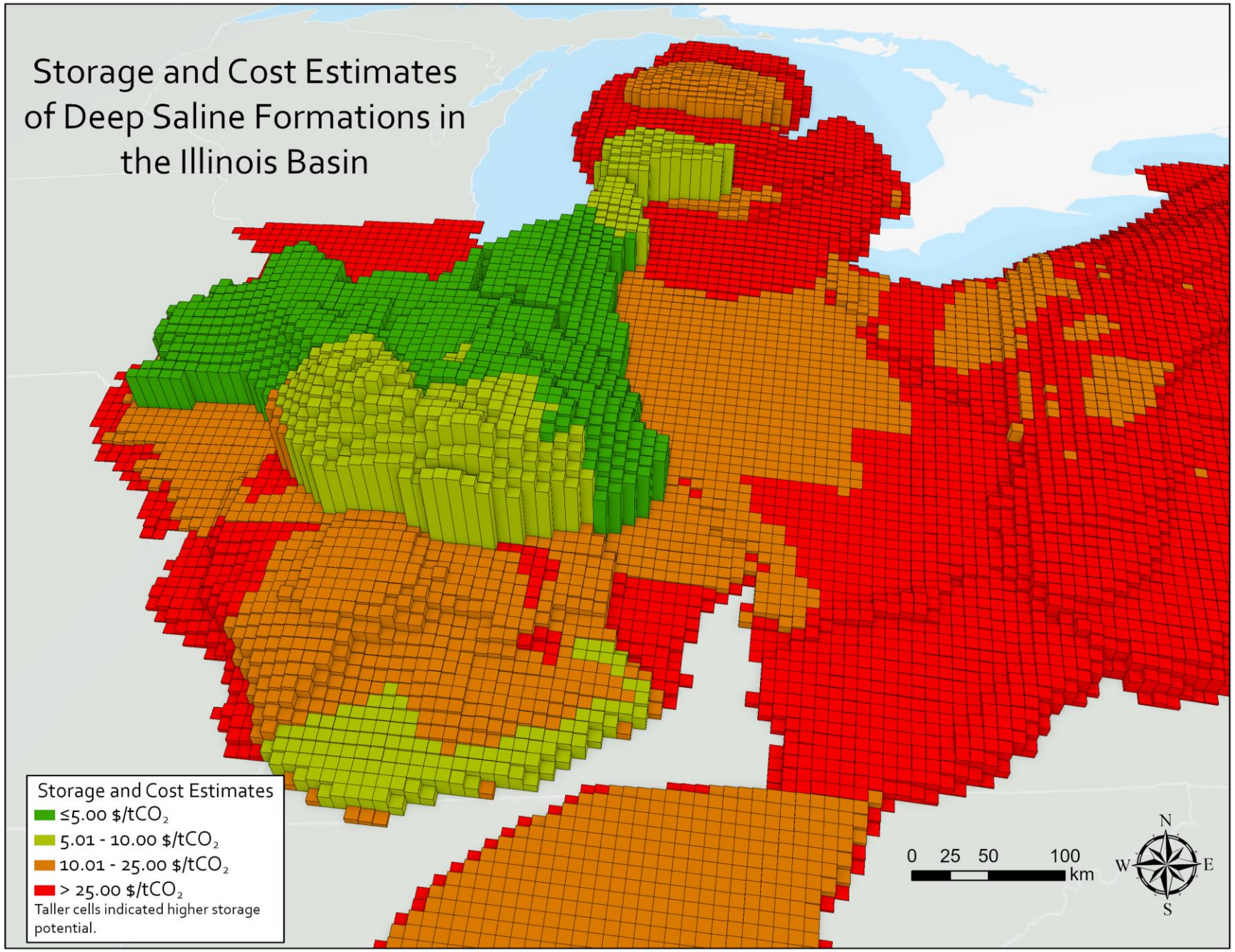
Middleton et al. (2020) Beam me up SCO_2T:Identifying geologic characteristics and operational decisions to meet global carbon sequestration goals, *Energy & Environmental Science*

BUILD: STORAGE

SCO_2T

National storage

- Coupled SCO_2T database & SCO_2T tool.
- Dynamic injection/storage, not volumetric analysis.
- SCO_2T economics.
- Replicable, with uncertainty.
- Operational tool (e.g., well spacing, 1 $MtCO_2$/yr).
- Effect of brine treatment.
- **FUTURE:** nationwide understanding of CO_2 injection rates, storage capacities, & costs.



Middleton *et al.* (2020) Great SCO_2T! Rapid tool for carbon sequestration science, engineering, and economics, *Applied Computing & Geosciences*

SimCCS: CCS Infrastructure Decision Support

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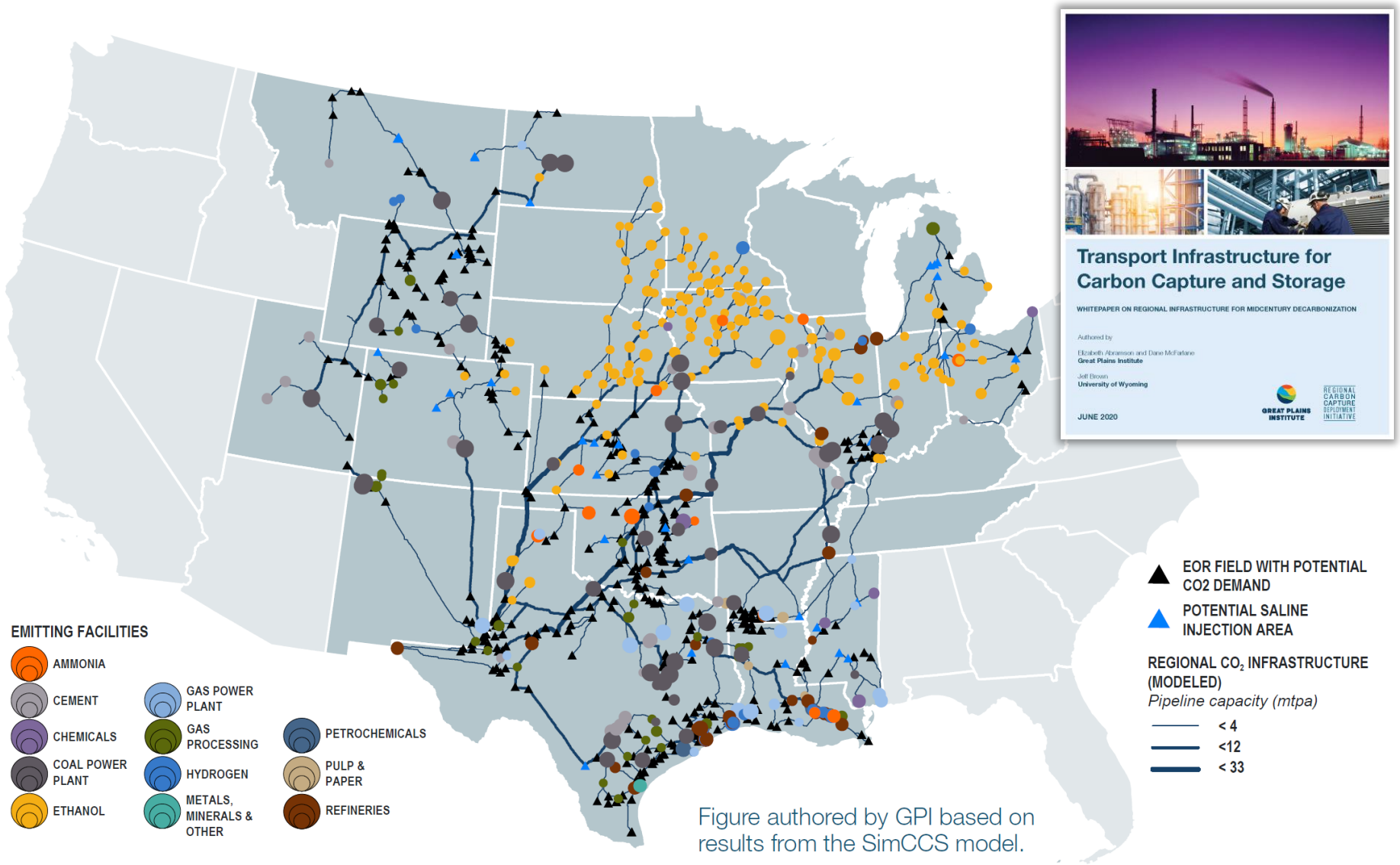


Figure authored by GPI based on results from the SimCCS model.

Gigatonne-scale CCS

- **US:** CCS scale of 100s $MtCO_2$/yr to 1+ $GtCO_2$/yr
- **GLOBALLY:** Scale of several gigatonnes.
- **APPROACH:** Planning, financing, policy, risk assessment, de-risking investment, outreach…

Great Plains Institute

The **REGIONAL CARBON CAPTURE DEPLOYMENT INITIATIVE** is a network of 25 states, and growing, that work together to help ensure near-term deployment of carbon capture projects that will reduce carbon emissions, benefit domestic energy and industrial production, and protect and create high wage jobs. The Initiative provides unique and valuable opportunities for governors, state officials, legislators, and other stakeholders to engage at the state, regional, and national levels.

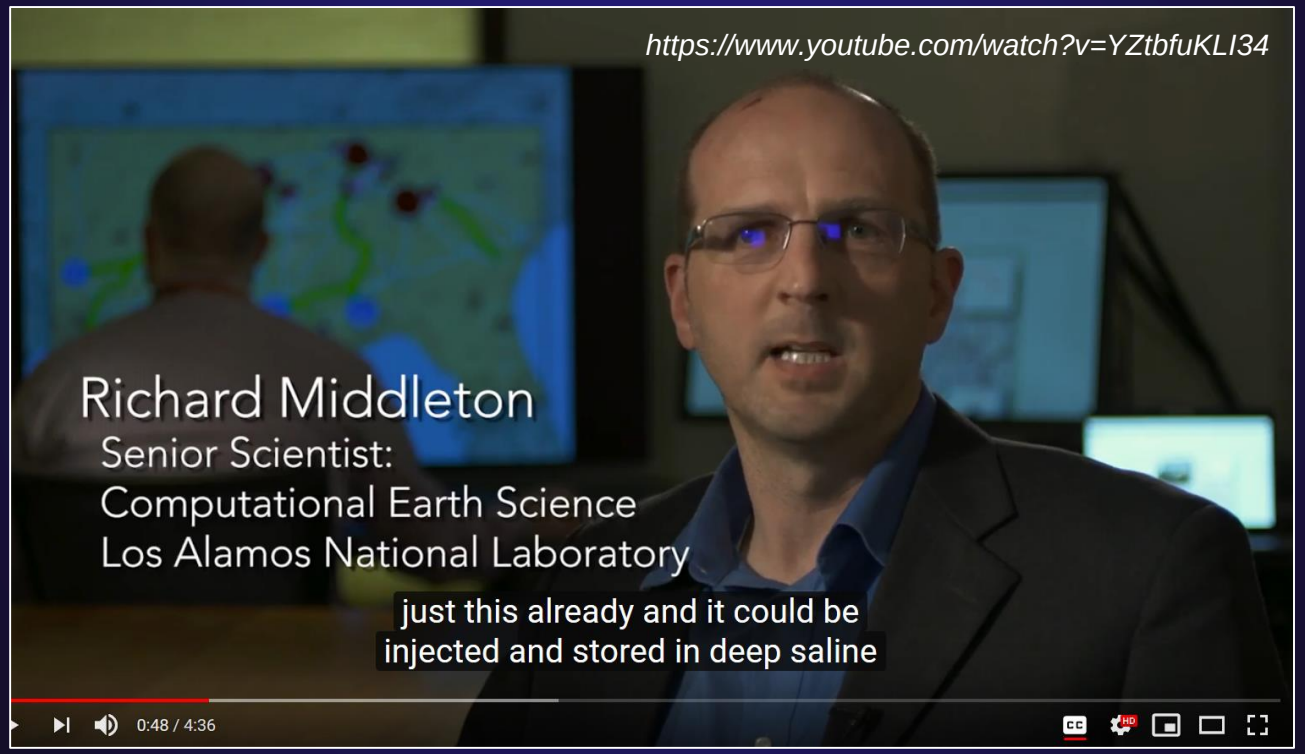
NEW ANALYSIS: Carbon Capture and Storage Infrastructure for Midcentury Decarbonization, https://www.betterenergy.org/blog/new-analysis-carbon-capture-and-storage-infrastructure-for-midcentury-decarbonization/

SimCCS: R&D 100

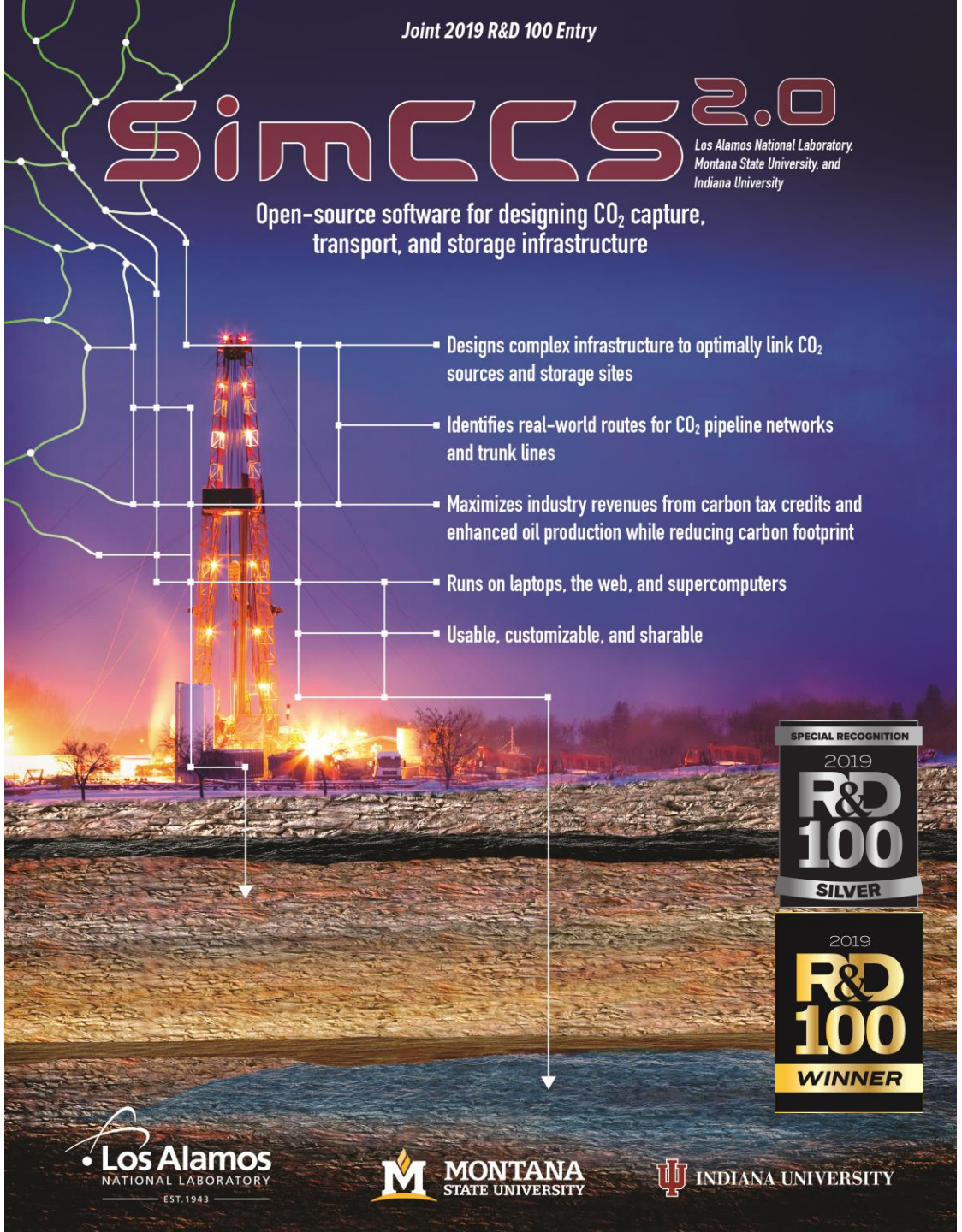
Two 2019 R&D 100 Award Wins

R&D 100 Awards: "Oscars of Industry"

- **R&D 100:** Software and Services.
- **Silver Medal:** Corporate Social Responsibility.



Charted Territory (2019) *SimCCS* wins two awards at the 2019 R&D 100 Awards, https://chartedterritory.us/2019/11/16/simccs-wins-two-awards-at-the-2019-rd-100-awards/



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Take Home Message

Synopsis

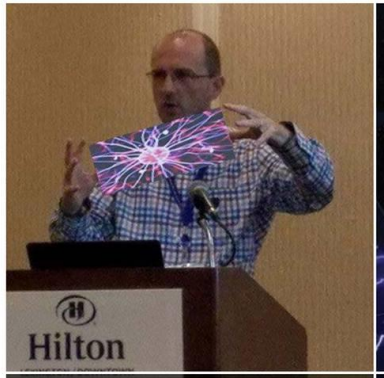
- Annual state of the *SimCCS* framework.
- FY20 outcomes.

Next-generation tools

- ***SimCCS*:** Decision-support for CCS infrastructure.
- ***NICO$_2$LE*:** CO_2 capture.
- ***CostMAP*:** CO_2 transport.
- ***SCO$_2$T*:** CO_2 storage.

Team *SimCCS*

- Data, tools & science development for CO_2 capture, transport, & storage.



How I think I look when giving a presentation

What the audience really sees