**SimCCS:** development and Applications

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Richard Middleton  *rsm@lanl.gov*

Earth and Environmental Sciences  
Los Alamos National Laboratory  
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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$T$: Identifying geologic characteristics and operational decisions to meet global carbon sequestration goals, *Energy and Environmental Science*, In Review.
SIMCCS: PROJECT HISTORY

Projects

   B. Nebraska Basin CarbonSAFE Integrated Pre-Feasibility Project | Sponsor: DOE | PI: Battelle (Duguid).
   D. CarbonSAFE Rocky Mountains Phase I: Ensuring Safe Subsurface Storage of CO₂ in the Intermountain West | Sponsor: DOE | PI: University of Utah (McPherson).
   E. Establishing an Early CO₂ Storage Complex in Kemper County, Mississippi | Sponsor: DOE | PI: SSEB (Nemeth).
   G. San Juan Basin CarbonSAFE Phase III: Ensuring Safe Subsurface Storage of CO₂ in Saline Reservoirs | Sponsor: DOE | PI: Mexico Institute of Mining and Technology (Balch).
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).
SIMCCS: BACKGROUND

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/

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Middleton et al. (2012) The cross-scale science of CO$_2$ capture and storage: from pore scale to regional scale, *Energy & Environmental Science*
**SimCCS Framework**

**Overview**

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

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Middleton et al. (2020) SimCCS: An open-source tool for optimizing CO₂ capture, transport, and storage, *Environmental Modelling & Software*
BUILD: CAPTURE

NICO\textsubscript{2}LE

Why?
• Identify commercial-scale CO\textsubscript{2} capture opportunities.

How?
• FUSE: data from EPA GHGRP/FLIGHT, EPA eGRID, RFA (ethanol)...
• Fuse: data from 15+ literature sources for CO\textsubscript{2} streams & capture costs.

What?
• GEODATABASE: source locations, CO\textsubscript{2} streams, & capture costs.
• SUPPLY CURVES: Identify economic opportunities.

Description:
NICO\textsubscript{2}LE database: CO\textsubscript{2} emissions for 16 categories across the United States. Data sourced from EPAGHG FLIGHT, EPA eGRID, and RFA ethanol data.

CO\textsubscript{2} emissions
- 0.25 MtCO\textsubscript{2}/yr
- 1 MtCO\textsubscript{2}/yr
- 10 MtCO\textsubscript{2}/yr

Middleton et al. (2017) Industrial CO\textsubscript{2} and carbon capture: near-term benefit, long-term necessity, Energy Procedia
**Why?**
- **NECESSITY:** Where, how, & cost of CO₂ 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.

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**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.

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Chen at al. (2019) Frankenstein’s ROMster: Potential Pitfalls of Reduced-Order Model Development in CO$_2$ Sequestration, IJGGC
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$_2$T: Identifying geologic characteristics and operational decisions to meet global carbon sequestration goals, *Energy & Environmental Science*
BUILD: STORAGE

**SCO₂T**

National storage

- Coupled SCO₂T database & SCO₂T tool.
- Dynamic injection/storage, not volumetric analysis.
- SCO₂T economics.
- Replicable, with uncertainty.
- Operational tool (e.g., well spacing, 1 MtCO₂/yr).
- Effect of brine treatment.
- **FUTURE**: nationwide understanding of CO₂ injection rates, storage capacities, & costs.

*Middleton et al. (2020) Great SCO₂T! Rapid tool for carbon sequestration science, engineering, and economics, Applied Computing & Geosciences*
**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...

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**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.
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.

Richard Middleton
Senior Scientist: Computational Earth Science
Los Alamos National Laboratory

just this already and it could be injected and stored in deep saline

https://www.youtube.com/watch?v=YZtbfuKLI34

**SimCCS**

**Take Home Message**

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

**Next-generation tools**
- **SimCCS**: Decision-support for CCS infrastructure.
- **NICO₂LE**: CO₂ capture.
- **CostMAP**: CO₂ transport.
- **SCO₂T**: CO₂ storage.

**Team SimCCS**
- Data, tools & science development for CO₂ capture, transport, & storage.