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Title: Developing CCUS system models to handle the complexity of multiple sources and sinks: An update on Tasks 5.3 and 5.4

Author(s): Middleton, Richard Stephen

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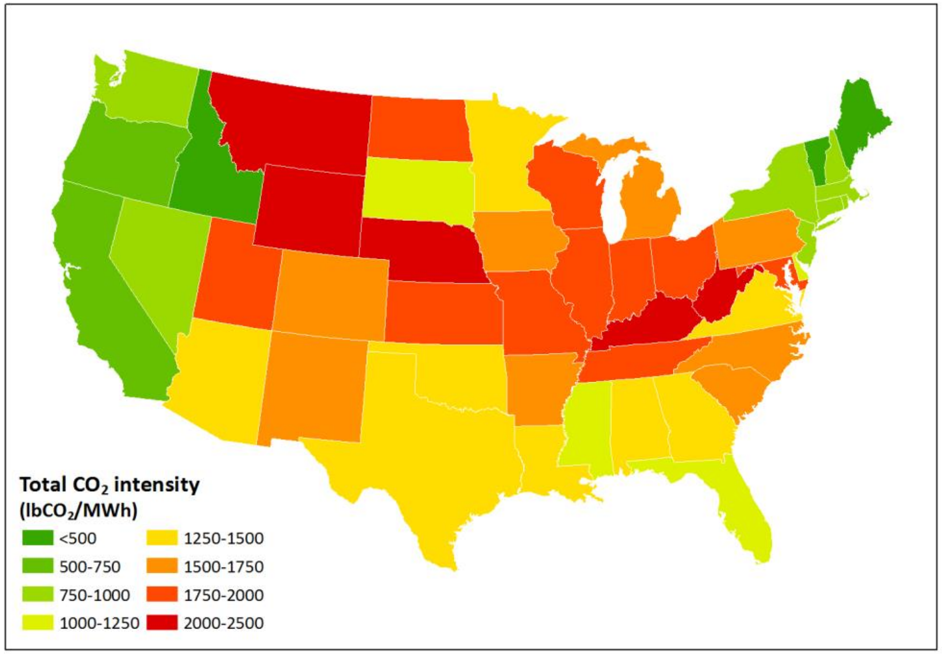
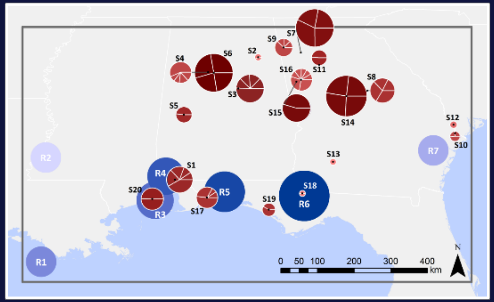
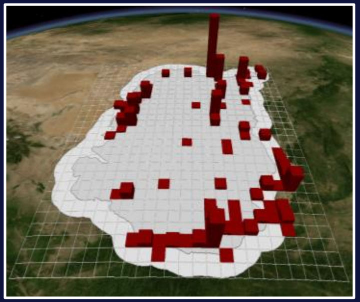
Developing CCUS system models to handle the complexity of multiple sources and sinks: An update on Tasks 5.3 and 5.4

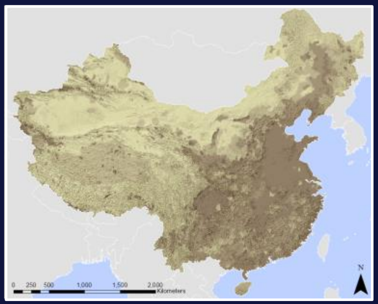
Richard S. Middleton
Los Alamos National Laboratory
rsm@lanl.gov

Kevin M. Ellett
Indiana University-Indiana Geological Survey
kmellett@Indiana.edu









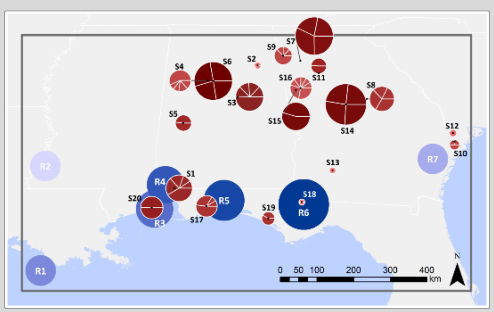
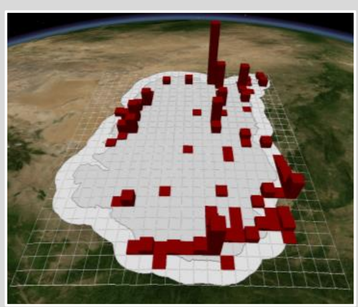
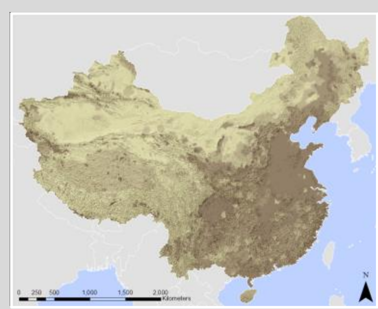
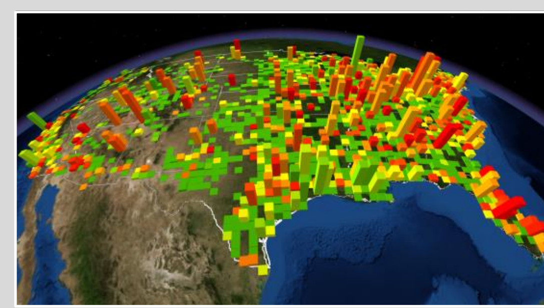
Multidisciplinary Problem, Multidisciplinary Team

Research participants

- ***Los Alamos National Laboratory:*** Richard Middleton, Philip Stauffer, Sean Yaw, Jing An.
- ***Indiana University– Indiana Geological Survey:*** Kevin Ellett, John Rupp, Ryan Kammer (LANL, Summer 2017), Yinzhi Wang (PhD student to post-doc, Summer 2017) .
- ***University of Wyoming:*** Ye Zhang and Zunsheng Jiao.
- ***New Mexico Institute of Mining and Technology:*** Evan Gragg (LANL, Summer 2017).
- ***Chinese Academy of Sciences:*** Jun Li, Bai Bing, Ning Wei, Xiaochun Li.
- ***Previous:*** The Ohio State University, University of Texas, Austin (DOE MLEF Program).

Industrial partners

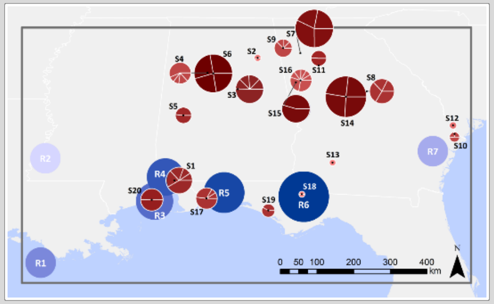
- **USA:** Southern Company, Duke Energy.
- **China:** Yanchang Group (EOR), Shenhua Group (CO_2 capture), Huaneng Group (EWR).

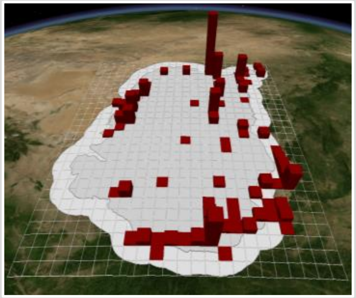





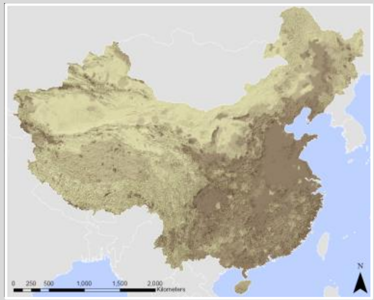
Theme 5: Overview

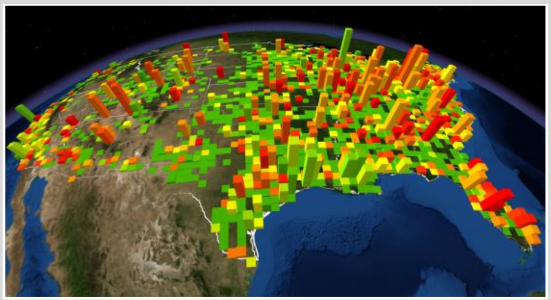
Theme 5: Systems Analysis and Modeling

1. Modeling the Impact of Power Plant Cycling and Developing Model-Based Optimal Mitigation Strategies, *West Virginia University.*
2. Collaborative Techno-economic Modeling of Combined IGCC and CCS, *Lawrence Livermore National Laboratory.*
3. Integrated Capacity Generation Decision Making for Power Utilities, *Los Alamos National Laboratory.*
4. A new Decision Support Tool for Integrated Assessment of CCUS, *Indiana University-Indiana Geological Survey.*









RECAP

Theme 5: Tasks 5.3 and 5.4

Task 5.3

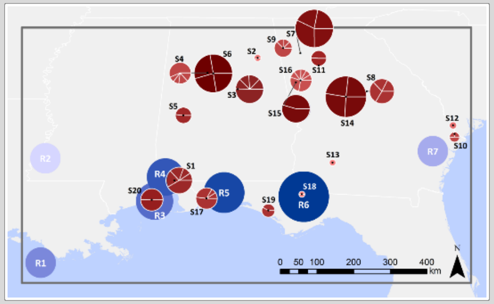
- Greater focus on CO_2 capture.
- Simultaneous understanding of electricity generation and CCS.

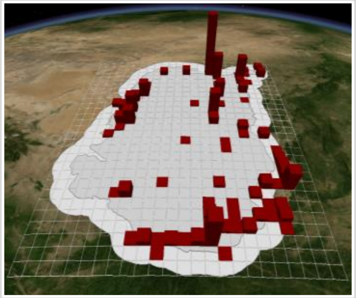
Task 5.4

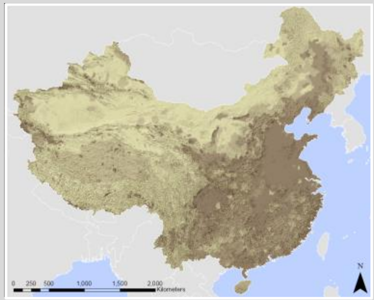
- Greater focus on CO_2 utilization & storage.
- Develop a next-generation decision tool to support CCUS decisions.

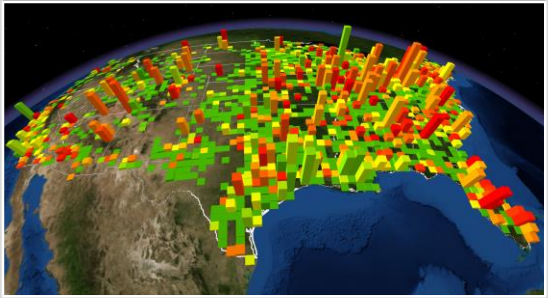
Task 5.3 & 5.4 objectives

- High level of synergy, using shared tool (i.e., *SimCCS/SimCCUS*).
- Integrate research outcomes across entire CERC.
- Identify project-wide targets and research gaps.
- Quantify and understand impact of uncertainty across CCUS decision space.









SimCCUS: Integrated CCUS Decision Framework

Los Alamos NATIONAL LABORATORY EST. 1943

DESCRIPTION

- coupled *economic-engineering* decision-making framework for CCS *scientists*, *stakeholders*, and *policy makers*
- understand how CCS technology—capture, transport, storage—could and should be deployed on an *industrial scale*
  - ***SimCCS**^CAP*: *cap-and-trade environment*
  - ***SimCCS**^PRICE*: *CO_2 tax*
  - ***SimCCS**^TIME*: *infrastructure evolution*

OPTIMIZATION ENGINE

Cost to open source, capture CO_2 + Cost to purchase land, construct pipeline, and transport CO_2 + Cost to open reservoir, inject CO_2

(1)	$x_{ij} - \sum_{d \in D} {}_{\max} Q^{p}_{ijd} y_{ijd} \leq 0$	$\forall i \in I, j \in N_i$	CO_2 flow must be less than maximum pipeline capacity
(2)	$x_{ij} - \sum_{d \in D} {}_{\min} Q^{p}_{ijd} y_{ijd} \geq 0$	$\forall i \in I, j \in N_i$	CO_2 flow must be more than minimum pipeline capacity
(3)	$\sum_{j \in N_i} x_{ij} - \sum_{j \in N_i} x_{ji} - a_i + b_i = 0$	$\forall i \in I$	CO_2 flow leaving a node must equal inflow
(4)	$a_i - Q^{s}_{i} s_i \leq 0$	$\forall i \in S$	CO_2 captured at a source must not exceed supply
(5)	$b_j - Q^{r}_{j} r_j \leq 0$	$\forall j \in R$	CO_2 stored at a sink must not exceed capacity
(6)	$\sum_{i \in S} a_i \geq T$		Target amount of CO_2 to store or sequester
(7)	$\sum_{d \in D} y_{ijd} \leq 1$	$\forall i \in I, j \in N_i$	Only one pipeline can be built between nodes

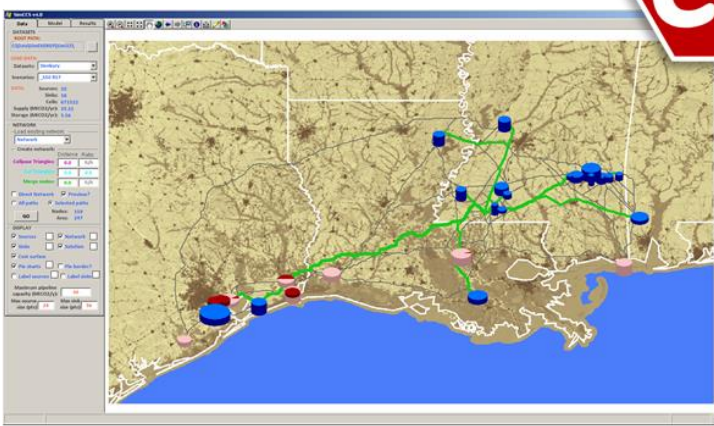
$y_{ijd} \in \{0,1\}$ $\forall i \in I, j \in N_i, d \in D$
$\in \{0,1\}$ $\forall i \in S$
$\{0,1\}$ $\forall j \in R$

0,1 constraints

$x_{ij} \geq 0$ $\forall i, j \in N_i$
$a_i \geq 0$ $\forall j \in S$
$b_j \geq 0$ $\forall j \in R$

Non-negativity constraints

INTERFACE

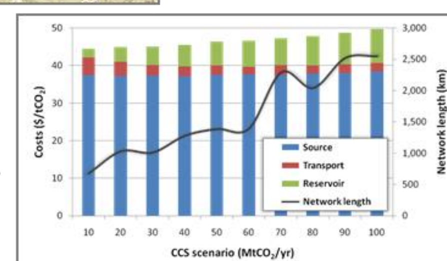


- custom/open-source GIS, network generation, model building

POLICY ANALYSIS

Spatial analysis

Economics & engineering

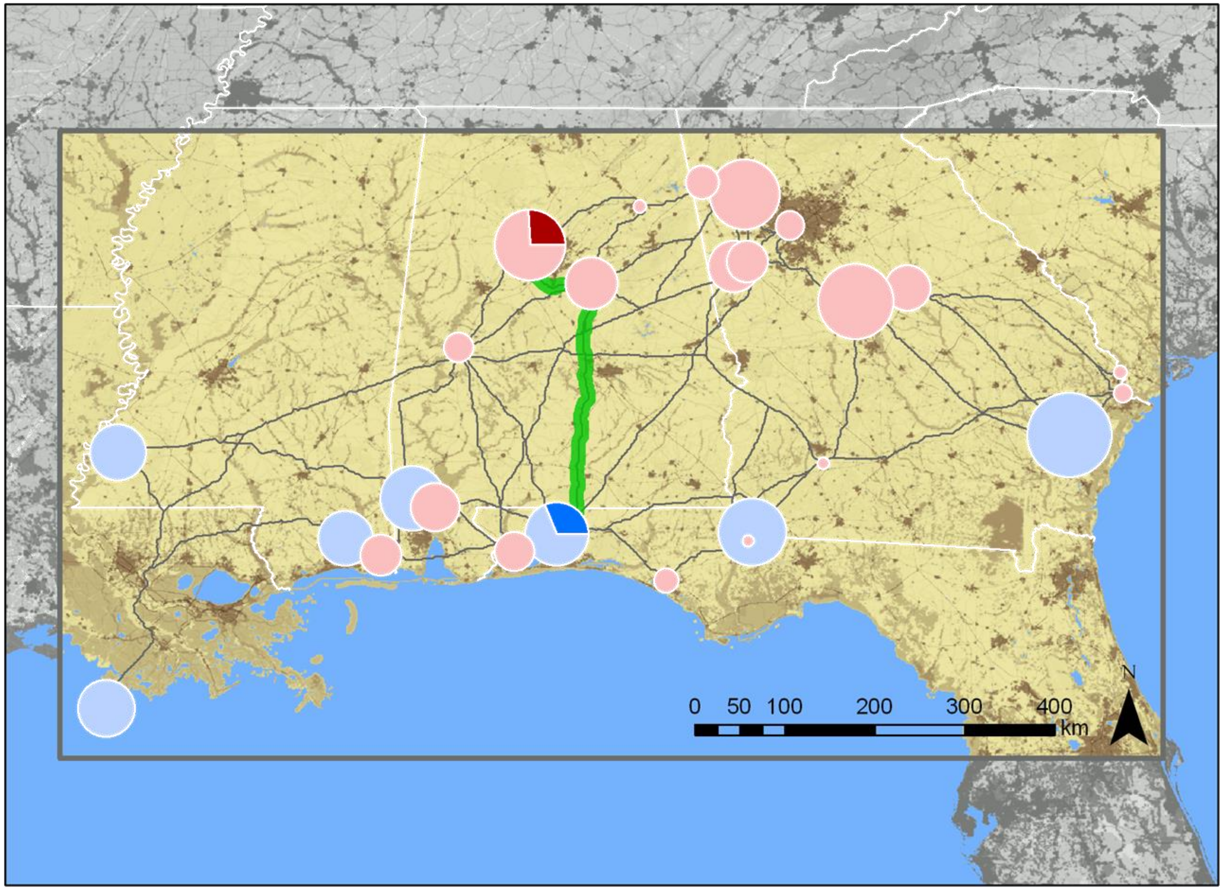


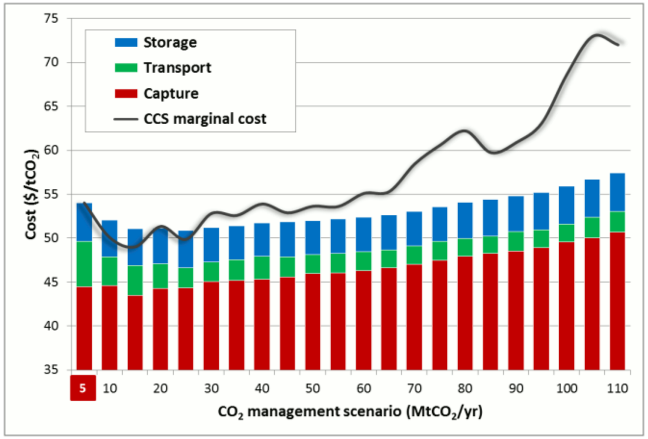
1 2 3 4 5 6 7 8 9 10 11 12 13

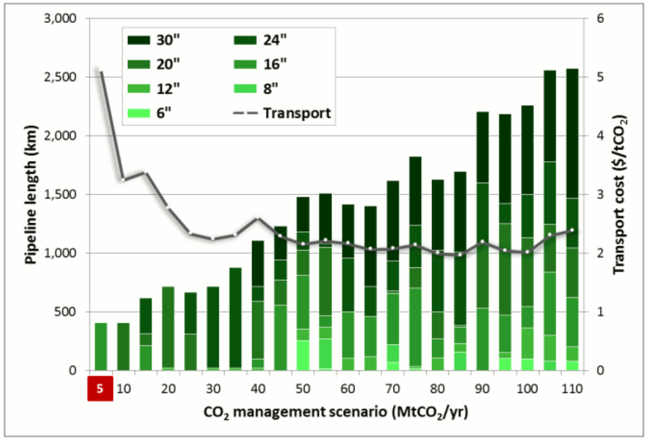
NNSA

SimCCUS: Integrated CCUS Decision Framework

- Capture costs & decisions drive economics.
- Considerable variability in the pipeline network and storage reservoirs.
- Significant economies of scale in the pipeline network.
- Multiple infrastructure thresholds.





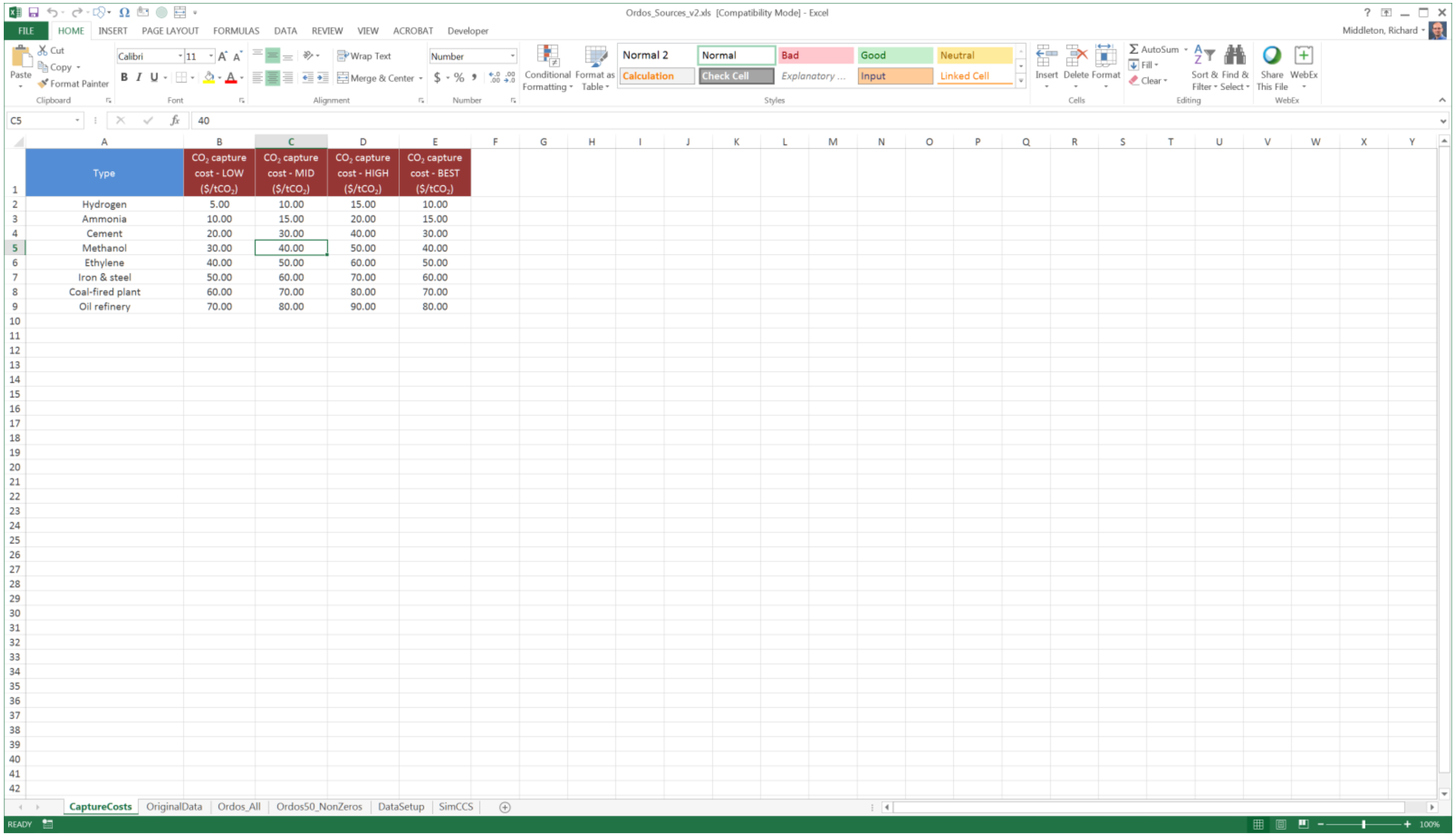


Middleton, R. S. et al. (2012). The cross-scale science of CO_2 capture and storage: from pore scale to regional scale. Energy & Environmental Science 5, 7328-7345

CO_2 capture costs

Develop CO_2 capture costs

- Power (coal-fired, gas) and industrial sources (e.g., iron & steel, methanol, etc.).
- Costs for United States and China.
- Applied in the Ordos Basin, China.



Type	CO_2 capture cost - LOW ($/t$CO_2$)	CO_2 capture cost - MID ($/t$CO_2$)	CO_2 capture cost - HIGH ($/t$CO_2$)	CO_2 capture cost - BEST ($/t$CO_2$)
Hydrogen	5.00	10.00	15.00	10.00
Ammonia	10.00	15.00	20.00	15.00
Cement	20.00	30.00	40.00	30.00
Methanol	30.00	40.00	50.00	40.00
Ethylene	40.00	50.00	60.00	50.00
Iron & steel	50.00	60.00	70.00	60.00
Coal-fired plant	60.00	70.00	80.00	70.00
Oil refinery	70.00	80.00	90.00	80.00

Next-generation CCUS Decision Making

New approaches

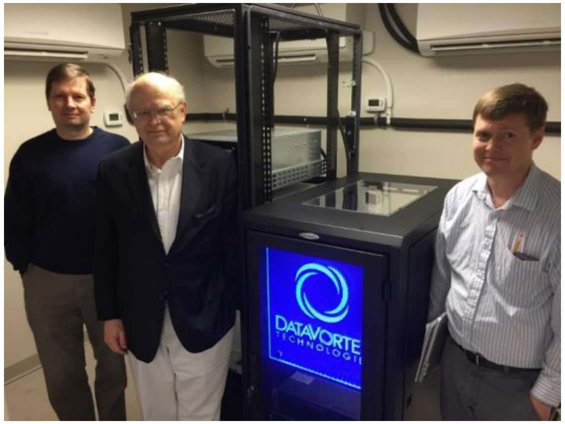
- Indiana University's Center for Research in Extreme Scale Technologies (CREST).
- Arizona State University (MS Thesis, Loy Lobo).

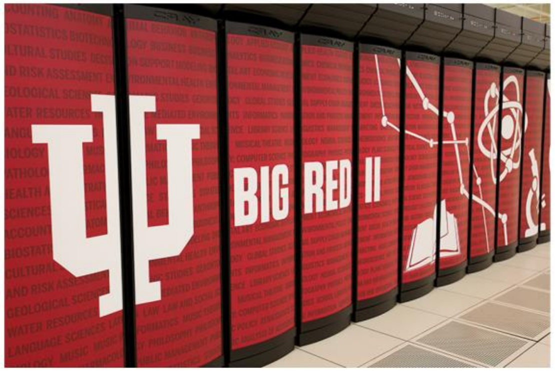
Workshop

- IU-CREST, March 2017
- Transition from desktop to high-performance computing (HPC) and open cloud-based solutions.
- Novel solutions processes for desktop and HPC.
- Target 1000x solution time improvement.
- Science Gateway with a web interface to provide access to IU's cyberinfrastructure for *SimCCUS* users.
- Follow-on meeting: May 2017.

Progress

- Benchmarking stage.
- Develop benchmark datasets and solution pools.





Next-generation CCUS Decision Making

Benchmarking: Ordos Basin

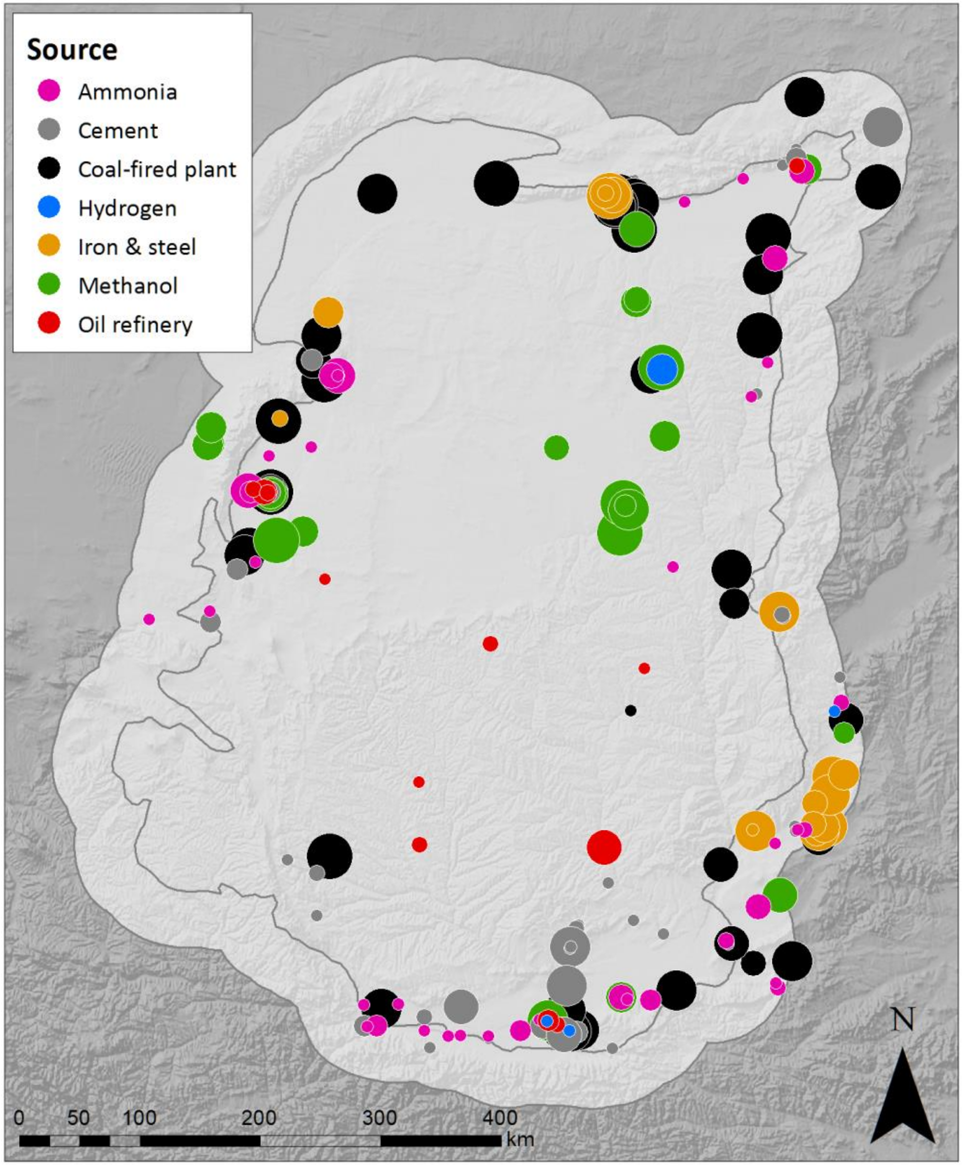
- Develop *SimCCUS* database for benchmarking.
- Problem inputs and solution times (based on existing technology).

Develop CO_2 source database

- Original data: partnership with Chinese Academy of Sciences (CAS).
- Clean and aggregate CO_2 data.

Develop CO_2 storage database

- Multiple partners: LANL, IU-IGS, CAS, UWYO.
- Identify storage sites based on pre-feasibility analysis.
- Calculate CO_2 parameters (LANL's *SCO_2T* tool) with known and estimate geologic parameters.



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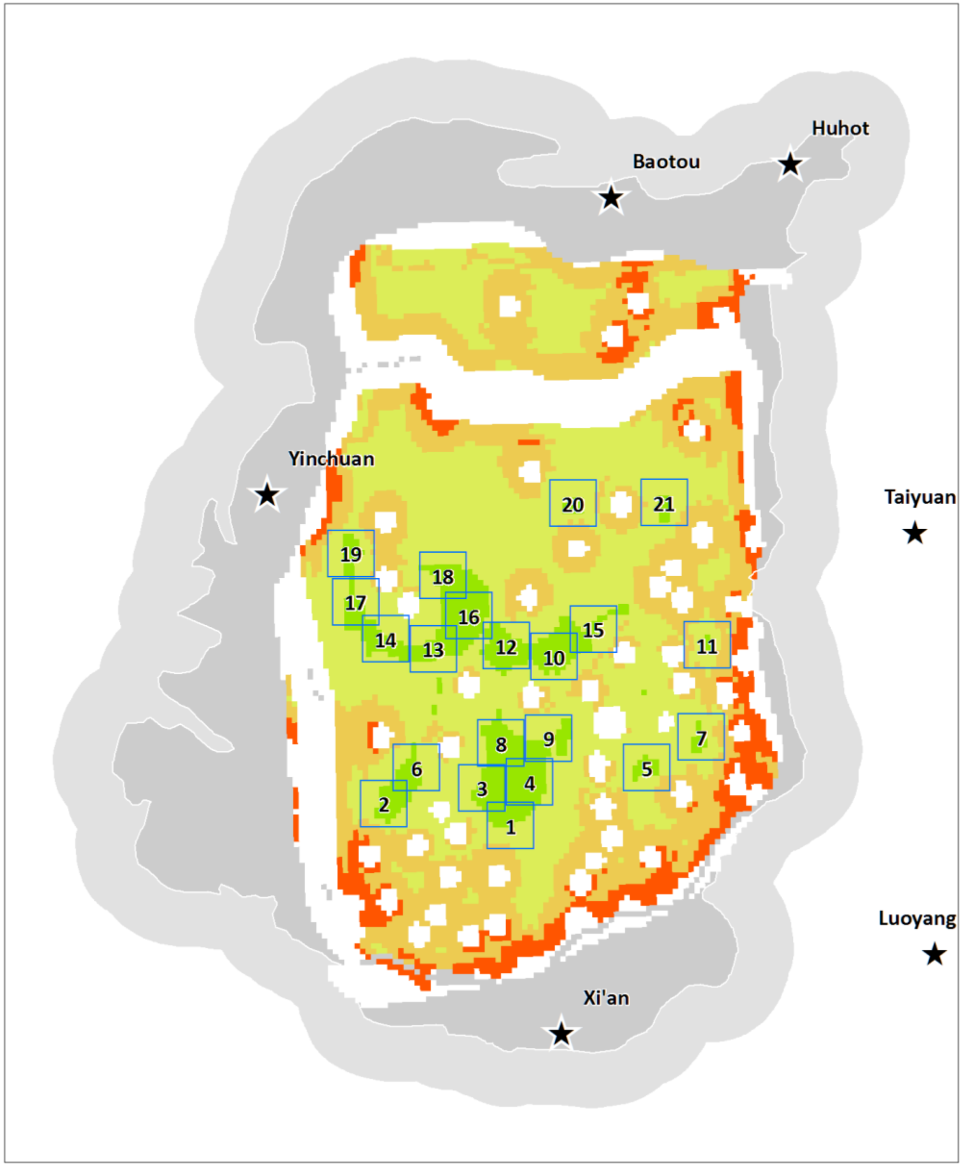


THRUST

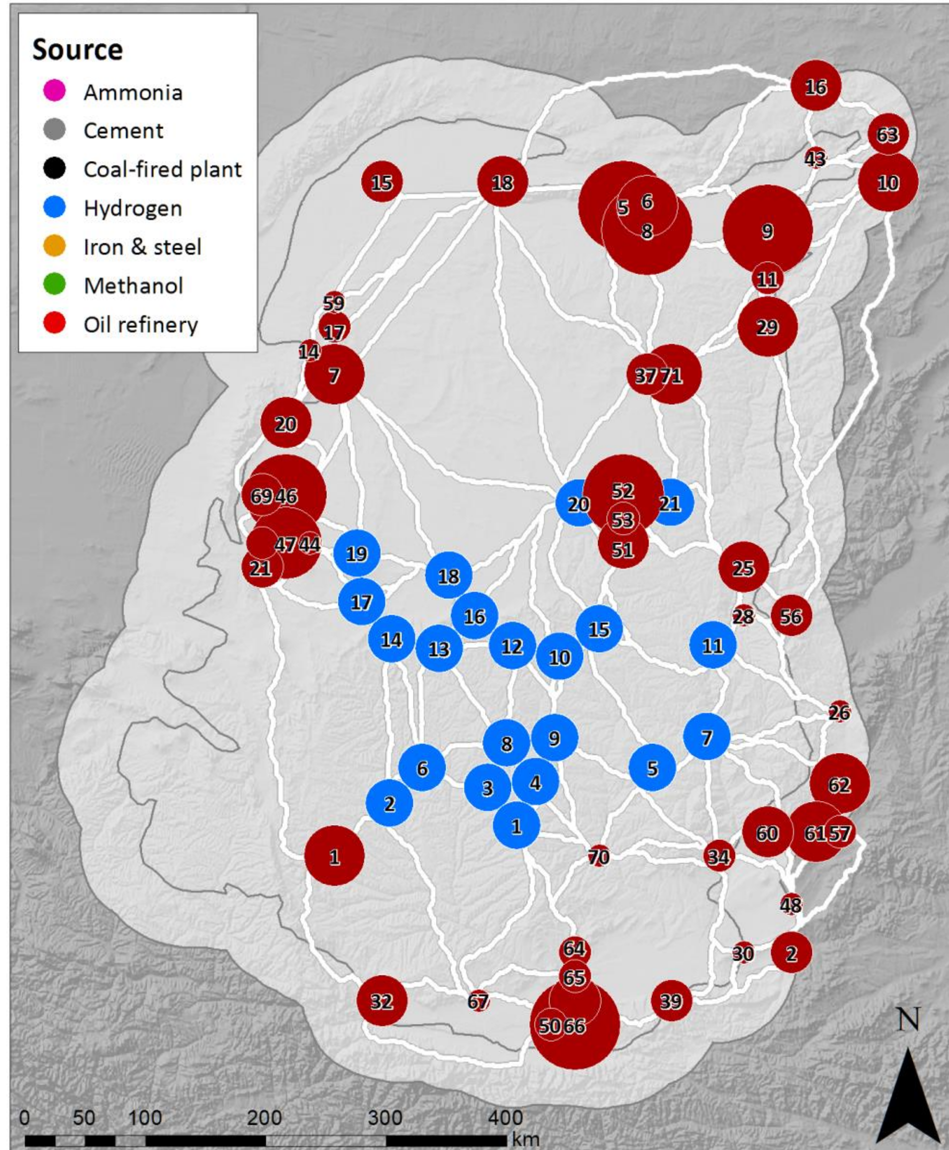
Next-generation CCUS Decision Making

Develop Potential Routes

- Connect sources (red) and sinks (blue) with a potential pipeline network.
- Shortest routes taking into geography (slope/aspect, land cover, population, river-rail-road crossings).

Benchmark solutions

- Solve *SimCCUS* using off the shelf software (IBM's CPLEX) using 1 and 24 threads.



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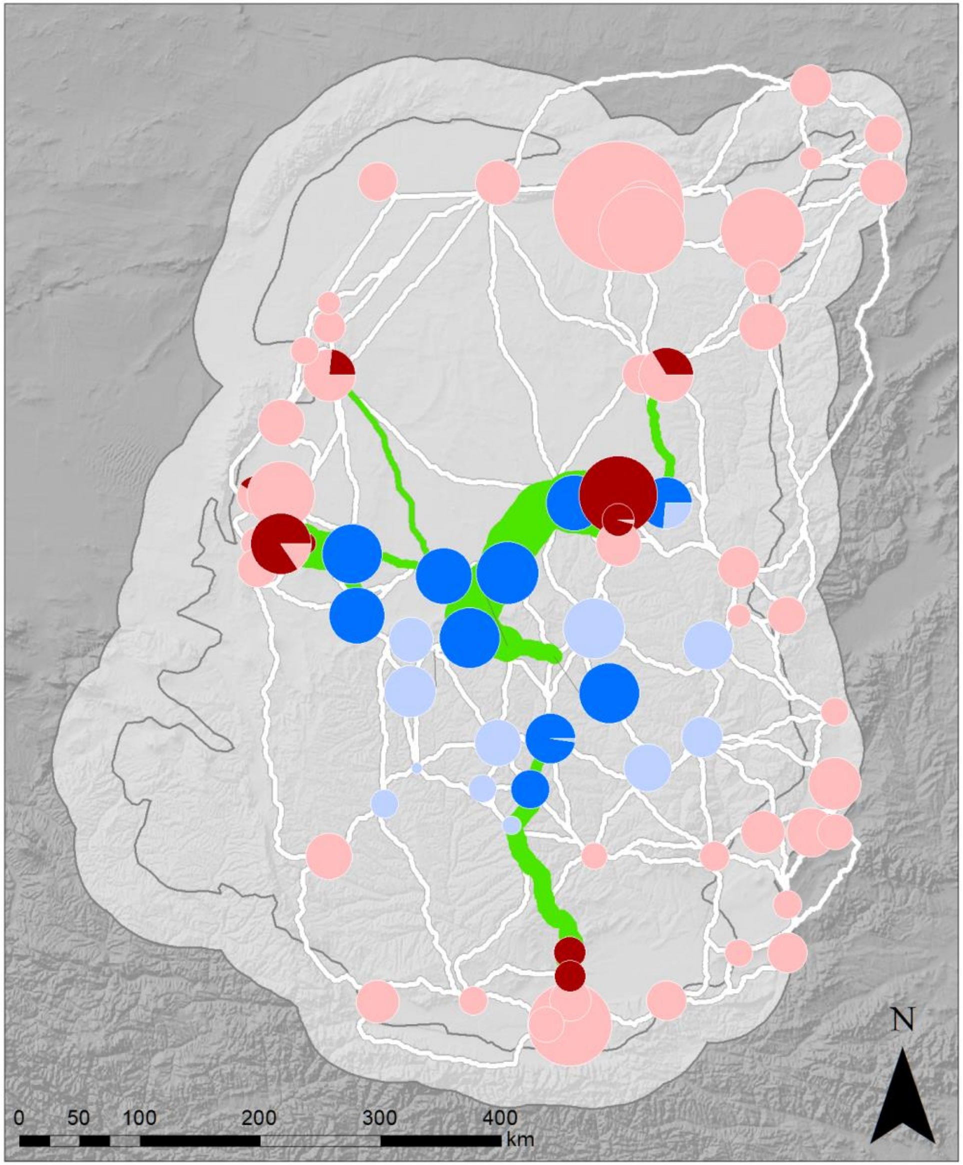

Project Timeline

Ongoing (Q2: April to June, 2017)

- Develop final CO_2 capture cost and storage/utilization database.
- Finalize *SimCCUS* solutions for the Ordos Basin and preliminary manuscript.
- Follow-on meeting with IU-CREST.
- Onboarding of new LANL postdoctoral researcher and summer fellows.

Planning (Q3: July to September, 2017)

- *SimCCUS* transition to Java in preparation for HPC and other novel approaches.
- Database development for the Southeast US regional study.
- Anticipated: *SimCCUS* workshop to be held in conjunction with the ACTC Annual Meeting– Sep 11-12 or 16-17 at Indiana University (3 hours from UK).

Planning (Q4: October to December, 2017)

- Final *SimCCUS* transition to Java.
- Anticipated: HPC *SimCCUS*.