Utilizing Models Developed for Water Management and Risk during Carbon Storage to Improve Water Management during Unconventional Gas Exploration and Production

Enid J "Jeri" Sullivan[1] and Rajesh Pawar[2]
[1]Chemical Diagnostics and Engineering Group
[2]Computational Earth Sciences Group,
Los Alamos National Laboratory

EPA Wastewater and Modeling Workshop
April 18, 2013
Research Triangle Park, NC
LA-UR-13-22732

UNCLASSIFIED

Research Problems (EPA, 2011)

- Water Acquisition: *What are the potential impacts of large volume water withdrawals from ground and surface waters on drinking water resources?*
- Chemical Mixing: *What are the possible impacts of surface spills on or near well pads of hydraulic fracturing fluids on drinking water resources?*
- Well Injection: *What are the possible impacts of the injection and fracturing process on drinking water resources?*
- Flowback and Produced Water: *What are the possible impacts of surface spills on or near well pads of flowback and produced water on drinking water resources?*
- Wastewater Treatment and Waste Disposal: *What are the possible impacts of inadequate treatment of hydraulic fracturing wastewaters on drinking water resources?*

Modeling Processes Needed

- Pore and fracture scale (physics-based)
  - Interactions between drill/frac fluids and minerals
  - Salt dissolution and mineral precipitation
  - Wellbore effects, leakage
- System/site scale (process-based)
  - Process effects
  - Risks
  - Costs
- Reservoir and regional scale (physics and processes)
  - Hydrology
  - Salt Balances
  - Contaminant Transport (in saline/brackish systems)

CO_2 PENS (Predicting Engineered Natural Systems) Model

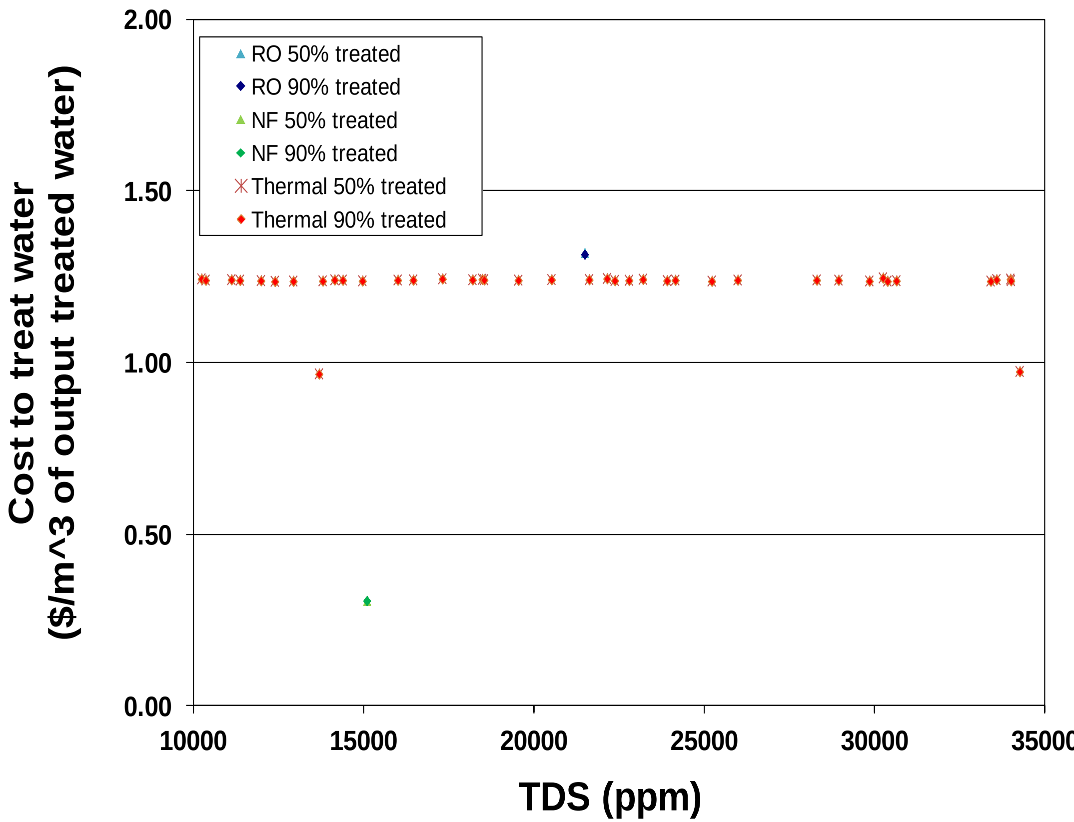
- Performance and risk assessment tool to analyze CO_2 and water movement at carbon storage sites
- Multi-realization, fixed and stochastic inputs, probabilistic simulations
- Numerical modeling of multiphase CO_2 flow and transport through porous rocks
- Individual process models abstracted to system framework, including:
- Field and numerical studies of migration and mixing of CO_2 in reservoirs and the atmosphere
- Optimization of surface pipelines for transport
- Lab and numerical studies of cement durability and effects on CO_2 storage (leaks).

Cost and process submodule of water extraction, treatment, disposal

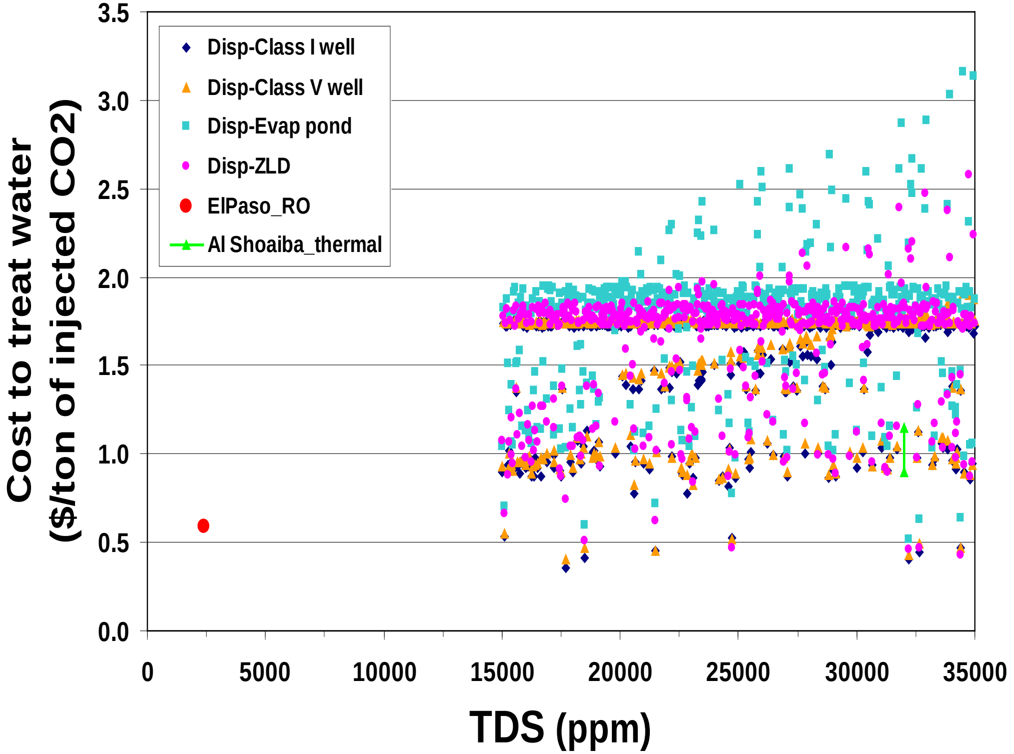
- 100-500 Realizations of each scenario in GoldSim™ module
- RO, NF, MED, and MSF treatment options
- 4 fixed cost of power ranges ($/kWh): 0.04, 0.07, 0.10, 0.20
- Variation in pH, turbidity, temperature, input salinity, desired output quality, treatment scenarios, and energy recovery (pressure)
- Fixed Feed volume (10 MGD or 37,854 m^3/d) (ranges possible)
- Two treated volume (% of feed volume) scenarios: 50%, 75%
- RO passes restricted to maximum of 3, otherwise cycles and costs accumulate until desired treated % of feed is reached
- Model selects correct pretreatments and treatments to use and applies cost data sets
- Model selects feasible concentrate disposal options and applies cost ranges.
- New addition: transport costs and organic pretreatment capability

Effects of different treatments on costs

- Cost to treat in $ per m^3 output treated water with constant injected CO_2 density
- Water volume normalized to 37,854 m^3 or 10 mgd
- Variable TDS (<35,000 mg/L)
- Variable T (15°C to 65°C)
- RO recoveries=50% and 90% of feed volume,
- Energy cost =$0.10/kWh,
- MSF thermal rate, no pressure recovery, no disposal included, 100 modeled realizations.



Cost effects of variable disposal methods

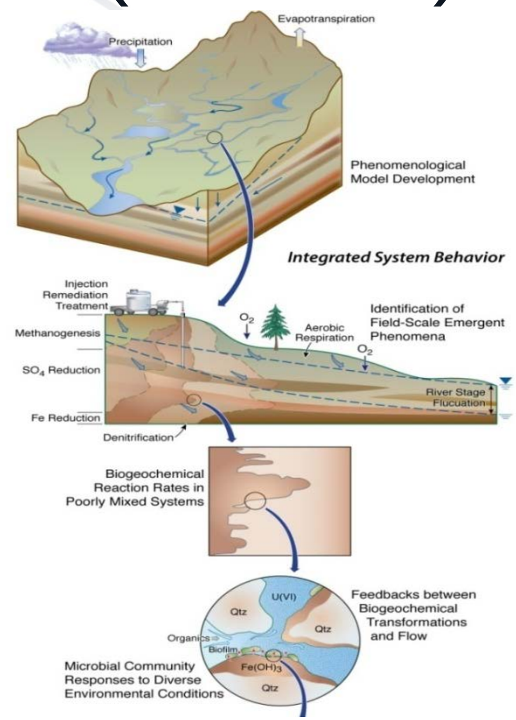


- Cost to treat in $/ton CO_2 injected
- Formation=Rock Springs (Weber)
- Variable TDS (15,000-35,000 mg/L)
- Variable T (10-117°C)
- Energy costs=$0.10/kWh
- MSF thermal method included
- Pelton pressure recovery
- 500 realizations.

UNCLASSIFIED

Advanced Simulation Capability for Environmental Management (ASCEM)

- **ASCEM** is a **state-of-the-art approach** for predicting contaminant fate and transport
- Based on a **modular, extensible, and open source** design that:
  - Leverages existing capabilities (many developed through SC-ASCR)
- Provides a dynamic and evolving **community platform** for testing and integrating new process-based understanding
- **'Born'** parallel for execution on emerging architectures
- **Integrates key tools into single framework**, including simulation, data management, visualization, parameter estimation and uncertainty quantification



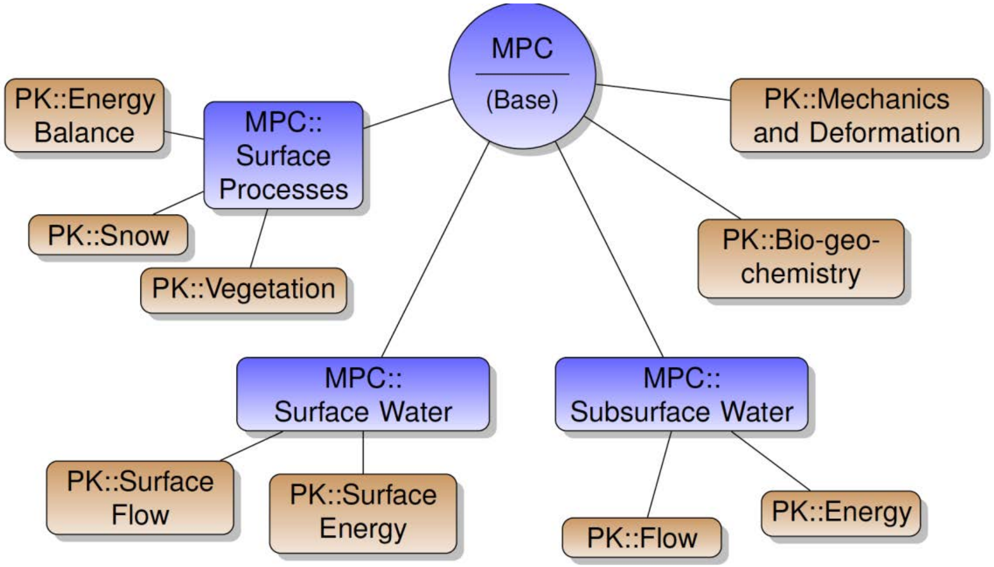
Wide Range of Complexity

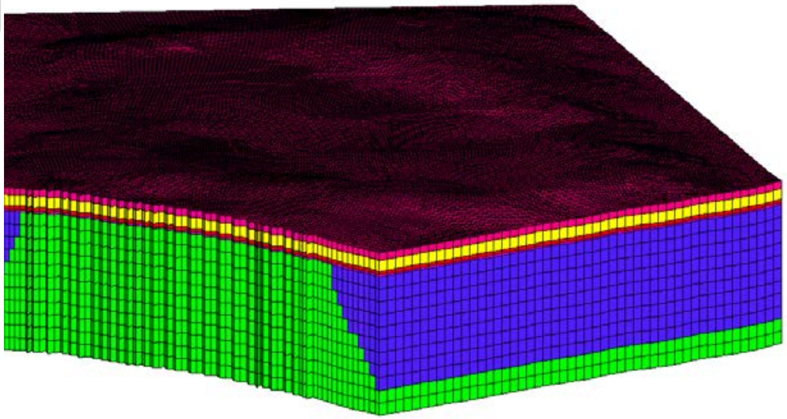
Wide Range of Platforms

UNCLASSIFIED

Predicting Climate Impacts and Feedbacks in the Terrestrial Arctic

- LANL laboratory-directed project leveraging ASCEM/Amanzi
- Goals are to predict future carbon releases in an evolving and topographically deforming landscape
- Requires flexible and extensible multiphysics simulation framework





Path Forward

- Continue and expand DOE, EPA, and industry collaborations for field and model studies
- Short-term: apply site-scale models of water treatment, transport, and disposal processes to hydraulic fracturing sites and needs, link to regional models (as per CO_2-PENS)
- Long-term: Utilize existing large-scale (high-performance) computational models developed for CO_2 storage, contaminant transport and hydrologic studies to evaluate impacts to drinking water quality and supplies over large scales and times >10 yrs.