EXPERIMENTAL DESIGN APPLICATIONS FOR MODELING AND ASSESSING CARBON DIOXIDE SEQUESTRATION IN SALINE AQUIFERS
DEFE 0004510

John D Rogers PhD, PMP, PE
Sigma Cubed Inc.

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and Building the Infrastructure for CO₂ Storage
August 12-14, 2014

(*Formerly Fusion Petroleum Technology Inc. Dba Fusion Reservoir Engineering Services Inc.)
OUTLINE

• Benefits to the program
  – Program Goals supported by project
  – Benefit of project to the program

• Project Overview
  – Goals and Objectives
  – Overview BP 1 efforts (completed)
    • Technical Review of BP 1
    • Key Findings of BP 1
    • Accomplishments BP 1
  – Goals and Objectives BP 2
    • Background Sigma Cubed Inc
    • BP 2 Overview and Technical Status
    • Accomplishments of BP2
  – Current Work
  – Project Accomplishments

• Summary
BENEFITS TO THE PROGRAM

• Program Goals Addressed in Project:
  1. Contributes to technical improvement of techniques to improve storage efficiency while ensuring containment effectiveness.
  2. Support of industries ability to predict CO₂ storage capacity in geologic formations to within ±30%

• Statement of Benefit
  - Successful demonstration of the modeling effort will illustrate that proxy type models can be developed to rapidly, cost effectively, and efficiently perform technical assessments of major engineering and scientific issues considered to be critical to the design, implementation, and operation of a saline aquifer CO₂ utilization and storage site.
Project Overview: Goals and Objectives

• Computer modeling effort to develop Proxy Models
  – Demonstrate feasibility of using ED/RSM techniques at field scale to optimize CO₂ sequestration process in brine aquifers and mature O&G fields
  – Determine effects of factors in CO₂ injection, capacity, plume migration, and seal integrity
  – Impurities of injected stream on reservoirs and seal
  – Rock types (e.g. dolomite and sandstones) petrophysical parameters
  – Geochemical effects of injected gas on brine and rock interactions
  – Well type configuration, construction, and placement

• Successful conclusion
  – is the ability to use commercial reactive transport simulator to model the coupled geochemistry and geomechanical effects listed above
  – Proxy models Developed
Project Overview  BP1 completed

- Objective: Define Static Reservoir model coupled with Reactive Transport Simulation
- Baseline Reservoir Simulation Model
  - Detailed realistic reservoir characterization model
  - Detailed Rock mineralogy/assemblage
- Commercial third party reactive transport simulator tested
  - Severe limitations of reactive transport simulation software for engineering purposes
  - Subsequent releases have attempted to rectify
From 14 interpreted faults and four horizons developed a six fault and four horizon structure model JewelSuite modeling software later modeled in Crystal with mineralogy.
Technical Review BP1 – Static and Dynamic Grid

• Reservoir Grid Development
  - 3.5 MM cell geologic grid
  - Lateral dimensions 107ft x 110ft x 2ft
  - Upscaled grid for simulator 144,018 variable cells roughly 500ft x 500ft x 2ft
Technical Review BP1 – Facies Zone 1
Technical Review BP1 – Facies Zone 2
Technical Review BP1 – Facies Zone 3
Permeability Model Layer 2 (Sundance)
Permeability Model Layer 18 (Sundance)
Permeability Model Layer 22 (Sundance)
Permeability Model Layer 35 (Crow Mtn)
Permeability Model Layer 58 (Crow Mtn)
Permeability Model Layer 62 (Crow Mtn)
Permeability Model Layer 70 (Alcova LS)
Permeability Model Layer 78 (Red Peak)
Permeability Model Layer 82 (Red Peak)
Permeability Model Layer 98 (Red Peak)
### Technical Review BP1 – Rock Assemblage

<table>
<thead>
<tr>
<th>Mineral Name</th>
<th>Chemical Formula</th>
<th>density g/cc</th>
<th>Lower Sundance wt%</th>
<th>Crow Mountain wt%</th>
<th>Alcova LS wt%</th>
<th>Red Peak wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Albite</td>
<td>NaAl(Si_3)O_8</td>
<td>2.61565</td>
<td>6.1</td>
<td>5.88</td>
<td>0.00</td>
<td>8.78</td>
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<tr>
<td>Anhydrite</td>
<td>CaSO_4</td>
<td>2.96338</td>
<td>1</td>
<td>0.02</td>
<td>1.08</td>
<td>9.17</td>
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<tr>
<td>Anorthite (plagioclase)</td>
<td>CaAl_2Si_2O_8</td>
<td>2.76025</td>
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<td>0.00</td>
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<td>Calcite (Auth Carb)</td>
<td>CaCO_3</td>
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<td>12.45</td>
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<tr>
<td>Chaledony (Chert)</td>
<td>SiO_2</td>
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<td>0.5</td>
<td>1.37</td>
<td>2.06</td>
<td>1.17</td>
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<tr>
<td>Chamosite-7A (Chlorite)</td>
<td>(Fe^{2+},Mg)_2Al<a href="OH">(AlSi_3)O_10</a>_8</td>
<td>1.61455</td>
<td>1.8</td>
<td>3.86</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
<td>Dolomite (Auth Carb)</td>
<td>(CaMg)(CO_3)_2</td>
<td>2.86496</td>
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<td>12.45</td>
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<td>12.50</td>
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<tr>
<td>Hematite</td>
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<td>2.87</td>
<td>0.00</td>
<td>0.80</td>
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<tr>
<td>Hydroxylapatite ***</td>
<td>Ca_5(PO_4)_3(F,Cl,OH)</td>
<td>3.14738</td>
<td>0</td>
<td>0.00</td>
<td>0.00</td>
<td>0.30</td>
</tr>
<tr>
<td>Illite (clay)</td>
<td>(K,H_2O)(Al,Mg,Fe)_2(Si,Al)_4O_10[(OH)_2,(H_2O)]</td>
<td>2.76307</td>
<td>1</td>
<td>7.25</td>
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<td>12.10</td>
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<tr>
<td>Ilmenite</td>
<td>FeTiO_3</td>
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<td>0.30</td>
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<tr>
<td>K-Feldspar (Orthoclase)</td>
<td>KAlSi_3O_8</td>
<td>2.55655</td>
<td>0.8</td>
<td>3.27</td>
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<td>Magnetite</td>
<td>FeO·Fe_2O_3</td>
<td>5.28078</td>
<td>0</td>
<td>0.30</td>
<td>0.00</td>
<td>0.60</td>
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<tr>
<td>Muscovite (Mica)</td>
<td>KAl_2<a href="OH">AlSi_3O_10</a>_2</td>
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<td>1.90</td>
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<tr>
<td>Pyrite</td>
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<td>0.00</td>
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<td>Quartz</td>
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<td>Tourmaline (Use Schorl)</td>
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<td>0</td>
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**Secondary Reactions**

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<tr>
<th>Mineral Name</th>
<th>Chemical Formula</th>
<th>density g/cc</th>
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<tbody>
<tr>
<td>Dawsonite</td>
<td>NaAl(CO_3)(OH)_2 (used as an antiacid)</td>
<td>2.42825</td>
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<tr>
<td>Fayalite</td>
<td>Fe_2SiO_4</td>
<td>4.39269</td>
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<tr>
<td>Goethite</td>
<td>α-FeO(OH)</td>
<td>4.26771</td>
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<tr>
<td>Gypsum</td>
<td>CaSO_4</td>
<td>2.3051</td>
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<tr>
<td>Kaolinite</td>
<td>Al_2Si_2O_5(OH)_4</td>
<td>2.59405</td>
</tr>
<tr>
<td>Magnesite</td>
<td>MgCO_3</td>
<td>3.00929</td>
</tr>
<tr>
<td>Siderite</td>
<td>FeCO_3</td>
<td>4.04667</td>
</tr>
<tr>
<td>Smectite-high-Fe-Mg</td>
<td></td>
<td>3.00777</td>
</tr>
</tbody>
</table>

Gleaned from Picard's Petrography publications and Fusion's Petrophysical (log) mineral analysis in wt%
Technical Review BP1 – Fluid and Mineral

Water equilibrium for each modeled formation of interest

Mineral Assemblage in Equilibrium with Water output from PHREEQC bulk vol% basis

<table>
<thead>
<tr>
<th></th>
<th>Molecular Weight g/g-mole</th>
<th>density g/cc</th>
<th>Lower Sundance</th>
<th>Crow Mtn</th>
<th>Alcova LS</th>
<th>Red Peak</th>
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<tbody>
<tr>
<td>Albite</td>
<td>262.223</td>
<td>2.61569</td>
<td>0.057369</td>
<td>0.05275</td>
<td>0.008609</td>
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<td>Anhydrite</td>
<td>136.1376</td>
<td>2.96338</td>
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<tr>
<td>Calcite</td>
<td>100.0892</td>
<td>2.70995</td>
<td>0.366271</td>
<td>0.110839</td>
<td>0.613739</td>
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<td>Chalcedony</td>
<td>60.0843</td>
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<tr>
<td>Chamosite-7A</td>
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<td>0</td>
<td>0</td>
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<td>Dawsonite</td>
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<tr>
<td>Dolomite</td>
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<tr>
<td>Gypsum</td>
<td>172.168</td>
<td>2.30511</td>
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<tr>
<td>Hematite</td>
<td>159.6922</td>
<td>5.27559</td>
<td>0.007008</td>
<td>0.020676</td>
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<tr>
<td>Hydroxylapatite</td>
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<td>0</td>
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<td>Illite</td>
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<tr>
<td>K-Feldspar</td>
<td>278.3315</td>
<td>2.55655</td>
<td>0</td>
<td>0</td>
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<tr>
<td>Kaolinite</td>
<td>258.1603</td>
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<td>0.006254</td>
<td>0.005434</td>
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<td>0.022018</td>
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<td>Magnesite</td>
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<tr>
<td>Magnetite</td>
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<tr>
<td>Muscovite</td>
<td>398.308</td>
<td>2.8307</td>
<td>0.021256</td>
<td>0.008406</td>
<td>0.001112</td>
<td>0.097353</td>
</tr>
<tr>
<td>Pyrite</td>
<td>119.967</td>
<td>5.01115</td>
<td>0.000383</td>
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<td>0</td>
<td></td>
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<tr>
<td>Quartz</td>
<td>60.0834</td>
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<td>0.275762</td>
<td>0.447104</td>
<td>0.229072</td>
<td>0.339845</td>
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<tr>
<td>Siderite</td>
<td>115.8562</td>
<td>4.04667</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
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<tr>
<td>Smectite-high-Fe-Mg</td>
<td>418.0803</td>
<td>3.00777</td>
<td>0.005517</td>
<td>0.020684</td>
<td>1.4E-11</td>
<td>0.051532</td>
</tr>
</tbody>
</table>

Values in molality moles/kg H2O

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Technical Review BP1 – Simplified Block or layer cake model

- 73x17x100 124,100 cells
  - Fully Implicit model
  - Initially run as batch reactor no problem
- Turn one well on
  - Convergence problem
- Smaller version (~2D version) extracted from this model
  - Convergence problem
- Uplayered from 100 layers to 43 layers
  - Same error occurred
- Take out all minerals and the model runs
Technical Review BP1 – Model Areal Approximation
Technical Review BP1 – LBL TOUGH2 Products

• **TOUGH2**
  - MP version massively parallelized

• **TOUGHREACT**
  - Comprehensive non-isothermal multicomponent fluid flow and geochemical transport simulator
  - Developed by introducing reactive geochemical transport into the framework of TOUGH2 v2
  - Disadvantage is that it is not parallelized and integrated with TOUGH2 and not TOUGH2-MP

• **iTOUGH2**
  - LBL program for parameter estimation, sensitivity analysis, and uncertainty propagation analysis
  - Based on TOUGH2
  - Provides inverse modeling capabilities for the TOUGH2 code
  - Parallelized
Accomplishments – BP1

- Baseline Reservoir Model Defined
- Detailed reservoir characterization model defined
- Detailed Rock mineralogy/assemblage defined
- Commercial third party reactive transport simulator tested
  - Base model not successfully run
  - Required to develop proxy equations
Key Findings/Conclusions – BP1

• Lack of a functional Commercially available fully coupled reactive transport simulator was an obstacle in moving forward on this project in BP1

• Evaluating, incorporating, and modifying (parallelizing) LBL TOUGHREACT is not part of scope of this project and would take additional resources and funding
Background Sigma Cubed Inc.

- During BP1 Purchased FPTI (and subsidiaries FRESI) Feb 2011
- Delivers integrated reservoir solution services
- Bridging Geosciences and Engineering
  - Geoengineering™
  - Completion Engineering (Pragmatic, Applied Geomechanics modeling)
  - Microseismic Acquisition, Processing, and Analysis
  - Borehole Seismic Imaging (VSP)
  - Reservoir Modeling & Geophysics
  - Pore Pressure and Geohazards
- Company Strategy Parallels BP 2 objectives
Goals and Objectives – BP2

- Objective: Geomechanics Emphasis
- Computer modeling effort to integrate well completions design of geomechanical stresses
  - Oil/gas CO₂ utilization and storage site
- Design Placement and completion of wells
  - Impacts of natural geologic barriers to flow
  - Injectivity, Capacity, plume migration and seal integrity in CO₂ utilization/storage site
- Parallel to Company Business Strategy
Project Approach – BP2

- **BP 2 – February 2013**
  - Reviewed at 2013 DOE CS R&D Project Review

- **Limited Geochemistry**

- **SuperNOVA – Internal Platform Integrating GeoEngineering subsurface data acquisition**
  - DOE DEFE0004510 initially a small but important aspect of this SuperNOVA.
  - Geomechanics Rock and Petro-physics work flow
  - Leveraged to develop the technical geomechanical R&D portion of the project
  - Develop methods and techniques for completions practices for wells in carbon utilization and sequestration sites primarily in storage of mature oil and gas fields
  - Well placement, stimulation techniques and workflows will be evaluated as scheduled in the original proposal
Rock Physics Modeling

- **Goal**: Produce *standard set* of reservoir properties using whatever logs are available

- **Purpose**: Create pseudo-logs and extrapolated data (via Kriging, etc.) for use in field studies, reservoir and frac simulators, and data analytics

- **24 permutations of six types of logs**
  - Gr
  - SP/resistivity
  - Density
  - Neutron
  - Acoustic
Quick Look Petrophysics

- **Velocity models:**
  - Tosaya and Nur, Brocher, Castagna, Gardner, Gardner (mod. Castagna), Han, Eberhart-Phillips

- **Gamma ray (Shale) correction methods:**
  - Linear, Larinov (tertiary and old fluids), Clavier, 3 Stieber methods.

- **Density models:**
  - Gardner (mod. Castagna), Brocher

- **Sonic Porosity Models:**
  - Wyllie Time Average, Raymer-Hunt, Raymer-Hunt-Gardner

- **Rule based log processing; includes five rules:**
  - $\gamma$
  - $\gamma, \rho$
  - $\gamma, \rho, \Delta t_c$
  - $\gamma, \rho, \Delta t_c, \Delta t_s$
  - $\gamma, \rho, \Delta t_c, \Delta t_s, \phi_N$
Well Log Blocking

- Blocks well logs independently or cascading.
- Observes well tops and forces zone boundaries at well tops.
- Users can enter additional control points to force zone boundaries.
- Runs multiple realizations with different Minimum Blocking Intervals and Maximum Deviation Tolerances in parallel.
- Determines the most realistic blocking that preserves fine details.
Wellbore Modeling
Project Approach – BP2

- End 2013 No longer a direct part of SUPERNOVA
- Uses layer cake model to emulate RMOTC
- Utilizes CMG reservoir simulator software
  - Reactive transport simulator (GEM GHG modules)
  - Geomechanical modeling software
  - CMOOST sensitivity and optimization modeling
    - Develop proxy models
- Limited geochemistry
  - 1-3 minerals have been modeled
    - Calcite
    - Anorthite, Kaolinite, Calcite
    - 7 aqueous components
Project Technical Status – BP2

- Very long run times single processor
  - Single processor 4.3 days
  - 8 core 17.1 hours
  - 24 core 13.29 hours (3-minerals) => 9.7 hrs (1-mineral)
  - Fully implicit model
  - No geomechanics
  - Optimized for 24 processors

- Explicit adoptive/implicit Model
  - Normally has convergence problems
  - ~1 hr run time (single mineral)
  - 1+ hr run time (3 minerals)
Project Technical Status – BP2

• Upscaled
  – Improved the speedup
  – Lost accuracy and high material balance error

• Geomechanics
  – Geostatistically populated grid
    • From well log data
      – Poisson ratio and Young’s modulus
      – Density maps
  – Initially 6 hour run time
  – Upscaled geomechanics grid => ~1 hour
  – Currently simulator allows geomechanical properties define within rock types
    • New release to have each cell populated
Project Accomplishments

• **BP1 Reservoir Static Models Defined**
  – Baseline Reservoir Model Defined
  – Detailed reservoir characterization model defined
  – Detailed Rock mineralogy/assemblage defined
  – Commercial third party reactive transport simulator tested

• **BP2 Rock Physics Models Defined for Geomechnics**
  – Rock Physics concepts workflow created
  – “Quick Look” Petrophysics analysis created
  – Well bore simulator developed
  – Layer Cake Base reservoir model successful
    • Limited geochemistry (1-3 minerals)
    • Geomechanics model implemented
    • Reasonable Base model run times
Current On Going Work

• Developing Fractured Reservoir Models
• Developing Well Completion Sensitivity optimization models
  – Dendritic or network models
  – Develop Proxy models
• Complete Project August 31, 2014
Summary

- Key Findings/Lessons learned
  - Industry still lacks a fast commercial reactive transport simulator capable of complex reservoir geochemistry coupled with a geomechanical simulator.
  - Limited number of minerals can be modeled. The maximum limit and method to effectively model reactive transport is unknown.
  - Industry is making progress but with no market driver the progress and acceptance of need will be exceptionally slow.
  - Geomechanical modeling simulation is fairly well defined and market driver in oil and gas is accelerating coupled geomechanical transport simulator.
END
Project Summary

Goals
- ED/RSM Proxy Model Demonstration
- Provide a structured approach to uncertainty to field development design parameters and well completion scenarios

Performance Period
- Original plan: Three phases in two budget periods; Sep 20, 2010; 19 months
- BP1 Extended to October 31, 2012 => January 31, 2013
- BP 2 February 1, 2013 to August 31, 2014

Budget: Total - $1,010,879
- BP 1 $578,221; BP 2 $432,879
- Gov't share - $808,702 Recipient share - $202,177; 20% cost share
- BP 2 increased cost share to 52% Fed and 48% Recipient

Status
- BP 1 Completed
- Project modification in BP 2 from geochemistry and limited geomechanics to emphasize geomechanics with limited geochemistry
- Project ends August 31, 2014
Organization Chart

Principal Investigator
John Rogers, Ph.D., PMP, P.E.
VP Operations FRESI

Co-PI
CTO SIGMA³

Seismic processing
Imaging analysis
modeling
Staff Geophysicist

Reservoir Modeling
Reservoir Engineer

Petrophysics
Staff Petrophysicist
Gantt Chart