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

DEFE 0004510

John D Rogers PhD, PMP, PE
SIGMA³ Integrated Reservoir Solutions, Inc.

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OUTLINE

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BENEFITS TO THE PROGRAM

- Simulation and Risk Assessment :Technologies that will support industries ability to predict CO_2 storage capacity in geologic formation to within ± 30%

By:

- Demonstrating field scale feasibility of using ED/RSM techniques to optimize engineering design and operational parameters for CO_2 sequestration process in brine aquifers using a commercial reactive transport simulator

Project Overview-Objectives

- Evaluate using a commercial reactive transport simulator
  - The migration of a CO_2 plume in a candidate reservoir to the effects of vertical and lateral heterogeneity, relative permeability and changes due to dissolution of the rock, pressure migration, fault distribution, and seal integrity;
  - The use of multilateral horizontal wells as opposed to vertical and/or single lateral wells;
  - Model the effects of competing thermodynamic and chemical effects within saline aquifers on the geologic formation and cap rocks by injecting impurities associated with the CO_2 gas stream;
  - The applicability of experimental design and response surface methods (ED/RSM) e.g. simultaneous impacts of parameter interaction

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Project Overview - Purpose or POC

Proxy objective function for CO_2 sequestration parameters using the Crow Mountain Aquifer the DOE RMOTC

1) Guide the data acquisition strategy during the early phases of field development of project [how the many geologic, rock and fluid properties interact in unison (rather than separately) that govern plume migration, injectivity, and reservoir capacity]

2) Provide inference of uncertainties with minimum number of simulations (how to integrate what is known and bridge what is unknown or uncertain of the many interacting parameters)

3) Provide a structured approach to uncertainty and carrying the uncertainties through to the field development plan, giving risked answers to development scenarios

4) Evaluate different well completions and construction techniques to optimize injectivity and ultimate capacity

5) Model the effects of competing thermodynamic and chemical effects within saline aquifers;

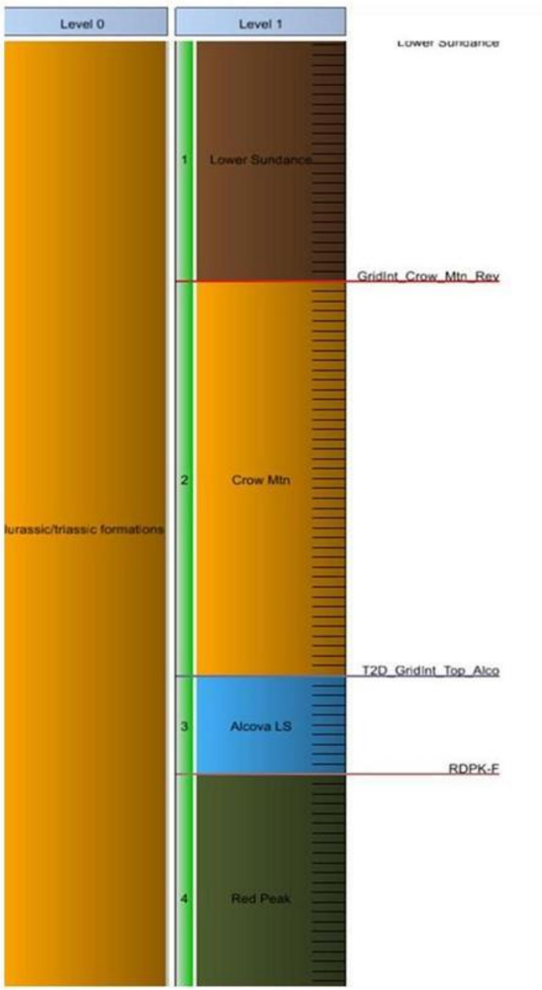
Project Overview –Why ED?

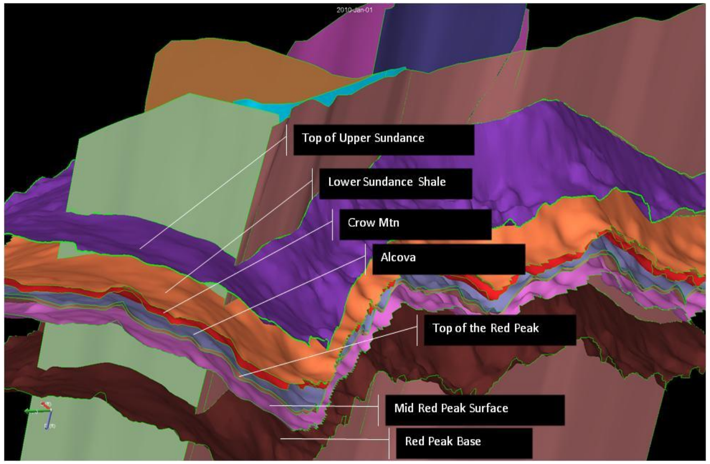
- Maximize information with limited resources
- Capture information not captured by changing one parameter at a time
- Today's software makes it easy to set up designs and analyze the results
- Represent a potential for significant time savings for the design and operations/management engineer
- Experimental design can contribute significantly in the operational decision making process
- Significant developments within the simulation industry to support this approach in the last 5-10 years
  - CMOST (CMG), MEPO / Decision (Scandpower), Couger (SLB), advancements in parallel computing etc.

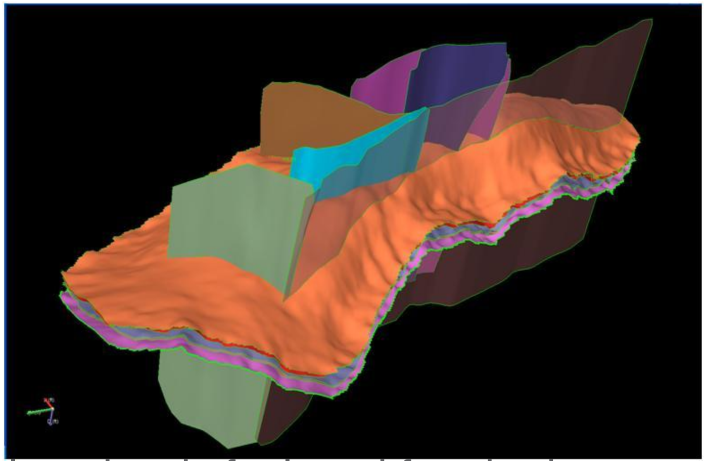
Project Overview -- Stratagem

- Built on Previous DOE project DEFE0001111
  - Sparse Seismic arrays in MVA
  - Obtain, process, evaluate realistic raw field seismic data
  - Crow Mountain brine formation US DOE RMOTC
  - Process data within FUSION
    - Time and Depth imaging
    - Integrated interpretation and analysis
    - Static and Dynamic Reservoir modeling
  - Evaluate reservoir pressures based on seismic data with geopressure concepts
    - Help in evaluation of seal breakdown and fracturing during CO_2 injection
    - PP, OB, FP, ES and respective gradients
    - Built a realistic reservoir model
- Use readily available commercial technical tools

Technical Status --Static Reservoir Model



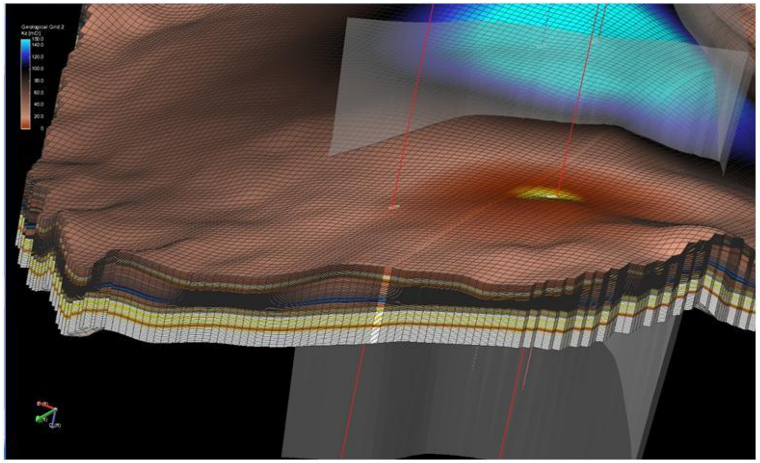


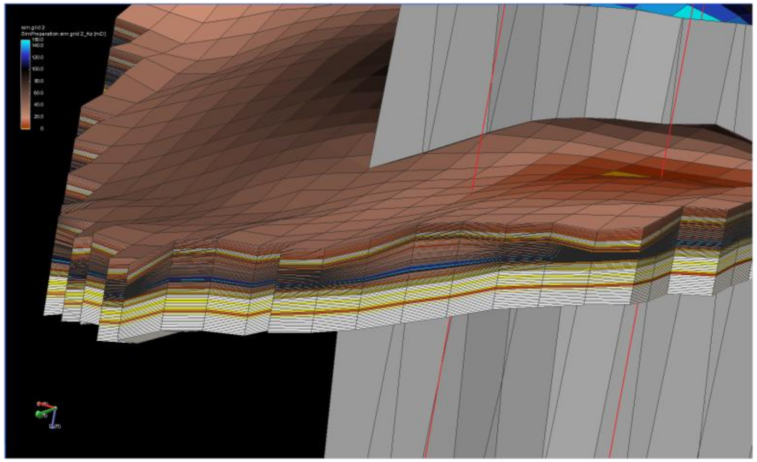


From 14 interpreted faults and four horizons developed a six fault and four horizon structure model JewelSuite modeling software later modeled in Crystal with mineralogy

Technical Status -- 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





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Technical Status-- Rock Assemblage

Mineral Name	Chemical Formula	density g/cc	Lower Sundance wt%	Crow Mountain wt%	Alcova LS wt%	Red Peak wt%
Albite	$NaAlSi_3O_8$	2.61569	6.1	5.88	0.00	8.78
Anhydrite	$CaSO_4$	2.96338	1	0.02	1.08	9.17
Anorthite (plagioclase)	$CaAl_2Si_2O_8$	2.76029	0	0.00	0.00	2.86
Calcite (Auth Carb)	CaCO3	2.70995	40.00	12.45	62.12	12.10
Chalcedony (Chert)	SiO_2	2.64829	0.5	1.37	2.06	1.17
Chamosite-7A (Chlorite)	$(Fe^{2+},Mg)_5Al(AlSi_3O_{10})(OH)_8$	1.61455	1.8	3.86	0	0.00
Dolomite (Auth Carb)	$(CaMg)(CO3)_2$	2.86496	18.10	12.45	13.08	12.50
Hematite	Fe_2O_3	5.27559	0.8	2.87	0	0.80
Hydroxylapatite ***	$Ca_5(PO_4)_3(F,Cl,OH)$	3.14738	0	0.00	0	0.30
Illite (clay)	$(K,H_3O)(Al,Mg,Fe)_2(Si,Al)_4O_{10}[(OH)_2,(H_2O)]$	2.76307	1	7.25	1.08	12.10
Ilmenite	$FeTiO_3$		0	0.30	0	0.60
K-Feldspar (Orthoclase)	$KAlSi_3O_8$	2.55655	0.8	3.27	0.00	1.43
Magnetite	$FeO{\cdot}Fe_2O_3$	5.20078	0	0.30	0	0.60
Muscovite (Mica)	$KAl_2(AlSi_3O_{10})(F,OH)_2$	2.8307	0.8	1.90	0.00	2.60
Pyrite	FeS	5.01115	0	0.00	0	0.10
Quartz	SiO_2	2.64829	29.1	47.47	20.59	33.72
Tourmaline (Use Schorl)	$NaFe^{2+}{}_3Al_6Si_6O_{18}(BO_3)_3(OH)_4$	3.244	0	0.60	0.00	1.18
Secondary Reactions						
Dawsonite	$NaAlCO_3(OH)_2$ (used as an antiacid)	2.42825				
Fayalite	Fe_2SiO_4	4.39269				
Goethite	α-FeO(OH)	4.26771				
Gypsum	$CaSO_4$	2.3051				
Kaolinite	$Al_2Si_2O_5(OH)_4$	2.59405				
Magnesite	$MgCO_3$	3.00929				
Siderite	$FeCO_3$	4.04667				
Smectite-high-Fe-Mg		3.00777				

Gleaned from Picard's Petrography publications and Fusion's Petrophysical (log) mineral analysis in wt%

Technical Status -- Fluid and Mineral Eq.

Water equilibrium for each modeled formation of interest

	initial	Lo Sundance	Crow Mtn	Alcova	Red Peak
pH	7.05	7.351835221	7.433680378	8.016824928	7.325966
H+	1.12E-07	4.45E-08	3.68E-08	9.62E-09	4.72E-08
Na+	0.12970	0.08180	0.06631	0.01767	0.08709
Al3+	1.37E-27	9.25E-18	4.56E-18	9.23E-20	1.13E-17
SiO2 (aq)	1.65E-25	0.0005708	0.0005708	0.0005708	0.0005708
Ca2+	0.004232	0.007336	0.002985	0.029580	0.008380
SO42-	0.028020	0.011770	0.000006	0.000000	0.010780
Fe2+	4.21E-10	5.47E-08	9.57E-08	7.04E-14	6.25E-08
Mg2+	0.000493	0.000264	0.000111	0.001068	0.000300
Fe3+	4.03E-18	5.98E-24	2.94E-24	5.98E-26	7.31E-24
HPO42-	1.62E-18	1.66E-18	1.90E-18	8.82E-19	7.32E-09
K+	0.001191	0.000041	0.000033	0.000009	0.000043
HS-	2.59E-18	2.74E-07	5.18E-07	0.00E+00	2.61E-07
Cl-	0.072760	0.071590	0.072280	0.073470	0.081170
values in molality moles/kg H2O					

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

	Molecular Weight g/g-mole	density g/cc	Lower sundance	Crow Mtn	Alcova LS	Red Peak
Albite	262.223	2.61569	0.057369	0.05275	0.000609	0.080925
Anhydrite	136.1376	2.96338	0.006898	0	0.009836	0.07835
Anorthite	278.2093	2.76029	0	0	0	0
Calcite	100.0892	2.70995	0.366271	0.110839	0.613739	0.128782
Chalcedony	60.0843	2.64829	0	0	0	0
Chamosite-7A	341.7688	1.61455	0	0	0	0
Dawsonite	143.9951	2.42825	0	0	0	0
Dolomite	184.4034	2.86496	0.153892	0.098897	0.122498	0.09455
Fayalite	203.7771	4.39269	0	0	0	0
Goethite	88.8537	4.26771	0	0	0	0
Gypsum	172.168	2.3051	0	0	0	0
Hematite	159.6922	5.27559	0.007008	0.020676	3.3E-13	0.00294
Hydroxylapatite	502.3214	3.14738	0	0	0	0.002387
Illite	383.9006	2.76307	0	0	0.008656	0
K-Feldspar	278.3315	2.55655	0	0	0	0
Kaolinite	258.1603	2.59405	0.006254	0.005434	1.29E-05	0.022018
Magnesite	84.3142	3.00929	0	0	0	0
Magnetite	231.5386	5.20078	0	0	0	0
Muscovite	398.308	2.8307	0.021256	0.088406	0.001112	0.097353
Pyrite	119.967	5.01115	0.000383	0.000122	0	0.000308
Quartz	60.0843	2.64829	0.275762	0.447104	0.229072	0.339845
Siderite	115.8562	4.04667	0	0	0	0
Smectite-high-Fe-Mg	418.0803	3.00777	0.005517	0.020684	1.4E-11	0.051532

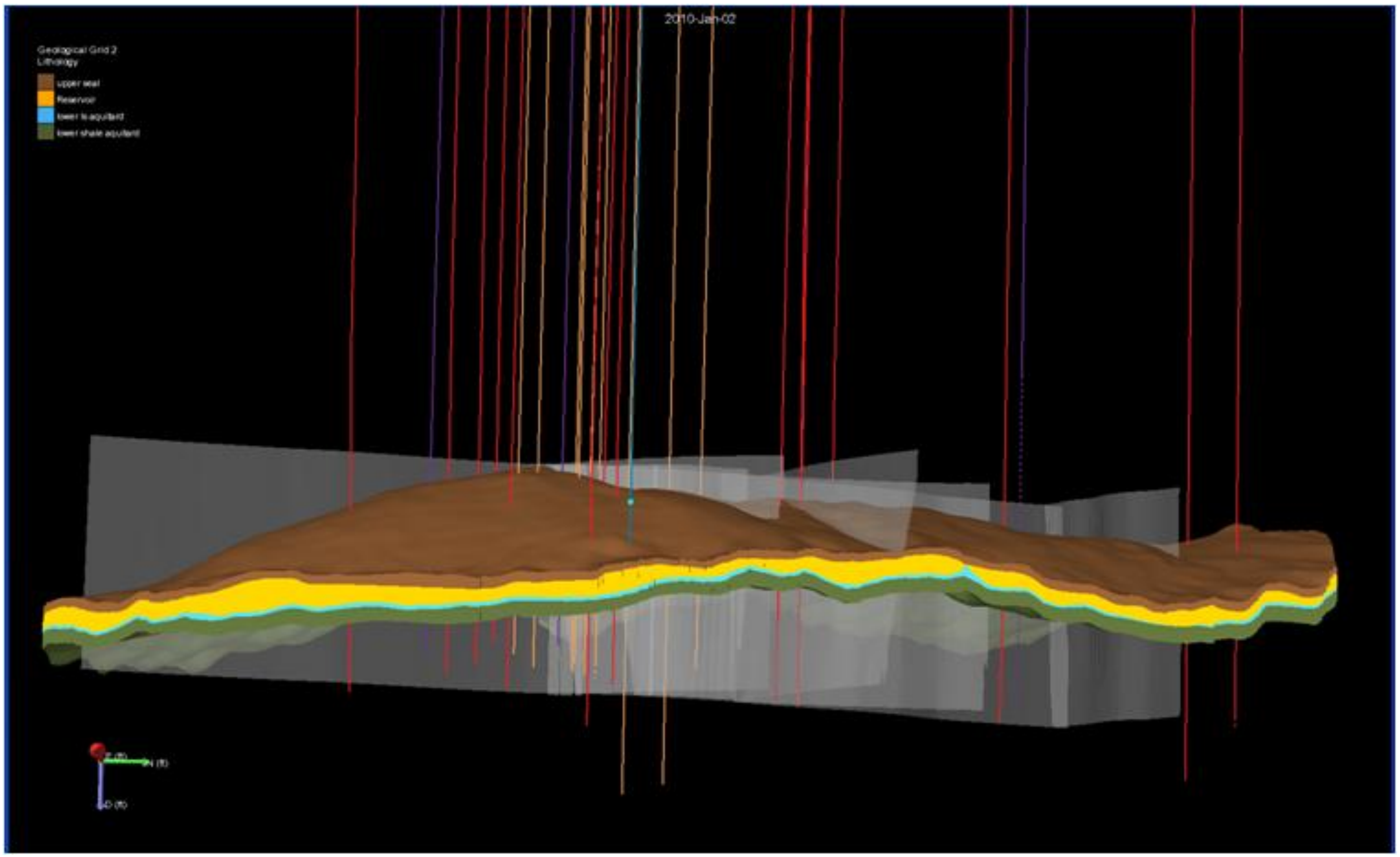
Technical Status -- Commercial Reservoir Simulator

- A very fast reservoir simulator having the capability of coupling geochemistry reactive flow is required for this project.
- CMG's GEM-GHG Multidimensional, finite difference, fully coupled reactive transport simulator (Geochemical model)
  – Parallelized
- CMOST is CMG's ED/RSM software that works in conjunction with CMG reservoir simulators
  – Sensitivity Analysis (SA)
  – History Matching (HM)
  – Optimization (OP)
  – Uncertainty Assessment (UA)

Technical Status -- Challenges

- CMG's Geochemistry GHG module doesn't work as advertised, promised, promoted and published
- Take the geochemistry requirement out and CMG-GEM and CMOST will work
  - This is just injecting CO_2 in an aquifer/reservoir which has been modeled over and over
- CMG is in the process of correcting the problem
  - A market driver for high priority is an issue
  - Indications are that it may be the end of 2012 before a fix is implemented --- if then

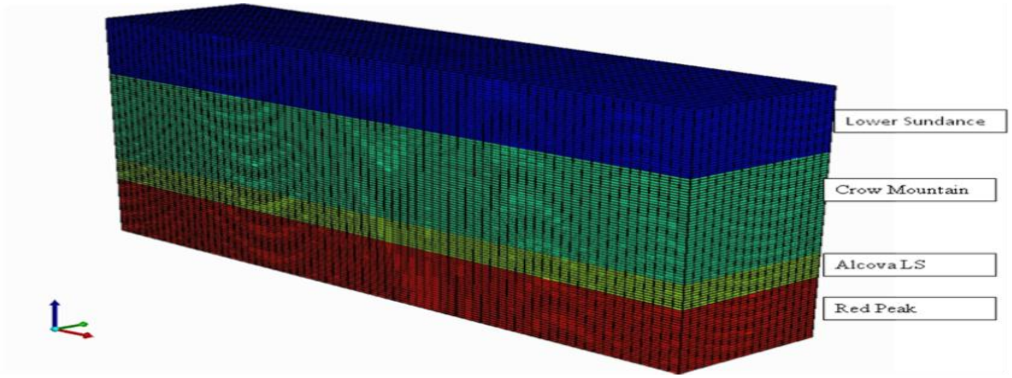
Technical Status -- Structured Reservoir Model



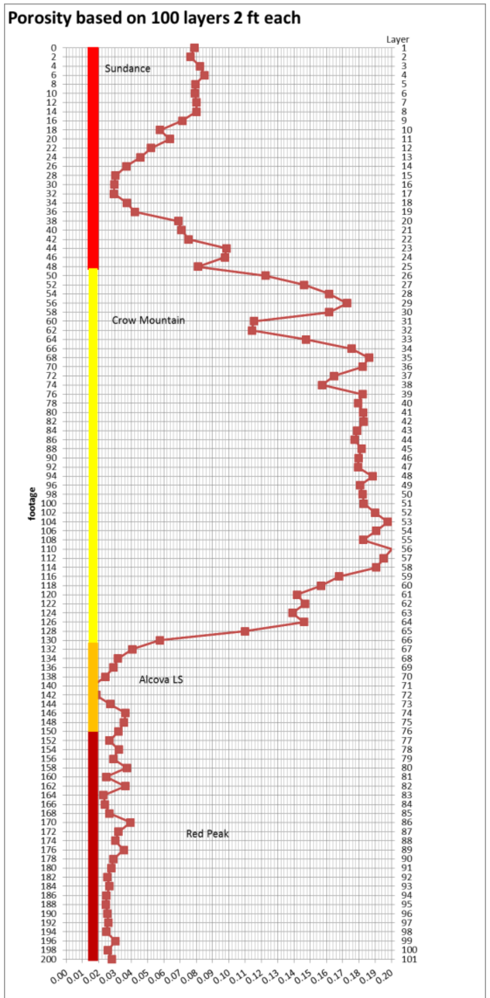
Lower Sundance (brown), Crow Mountain (yellow), Alcova (blue), Red Peak (green)

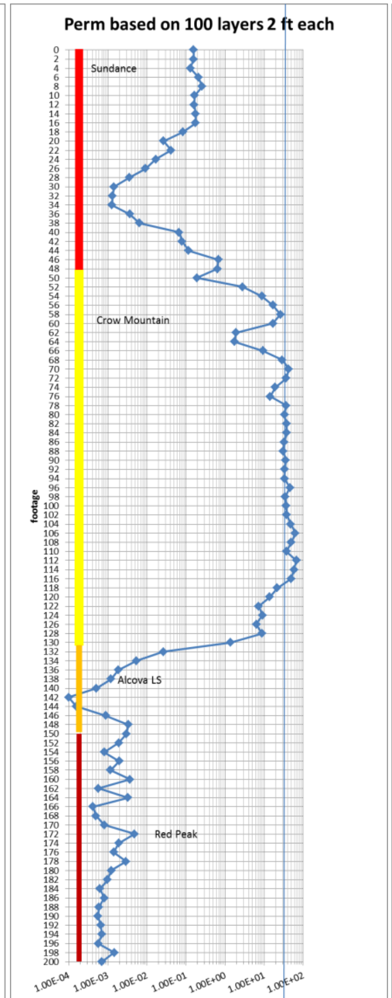
Technical Status -- Simplified Block or layer cake model

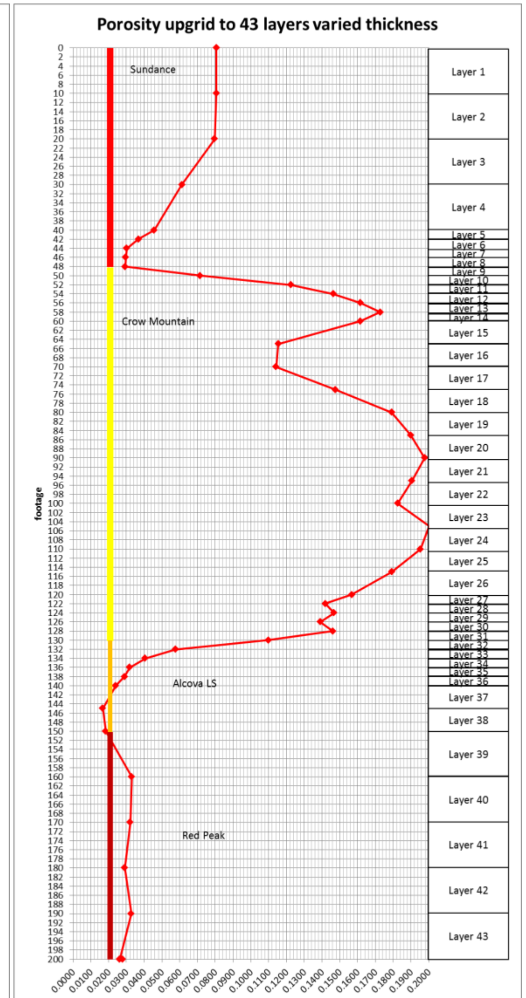
- 73x17x100 124,100 cells
  - Initially run as batch reactor no problem
- Turn one well on
  - convergence problem
- Smaller version (~2D version) extracted from this model
  - Convergence problem
- Uplayered from 100 layers to 43 layers
  - Same error occurred
- Take out all minerals and the model runs

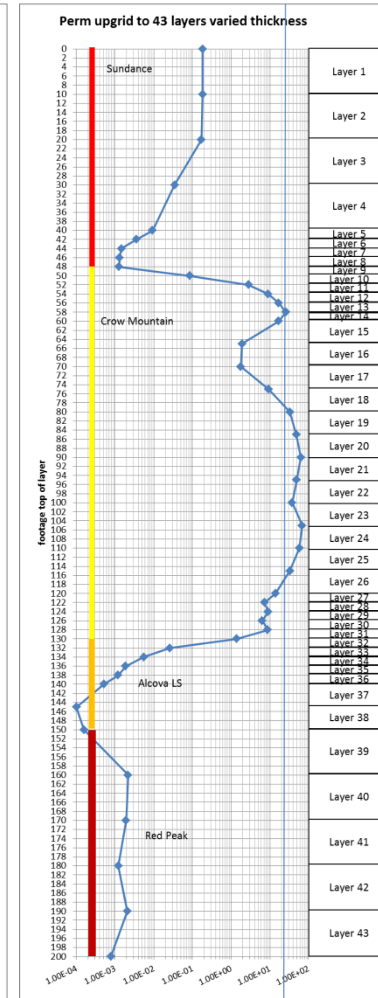


Technical Status -- Upgridding to Simpler Model









Technical Status -- Reactive Transport Simulators

- TOUGHREACT (LBL)
- CRUNCHFLOW (LBL)
- PFLoTran (LANL et al.)
- Nearly all do not allow the feasibility study as directly as needed by this project– with the exception of LBL TOUGH products

Technical Status -- 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
- *i*TOUGH2
  - LBL program for parameter estimation, sensitivity analysis, and uncertainty propagation analysis
  - Based on TOUGH2
  - Provides inverse modeling capabilities for the TOUGH2 code
  - Parallelized

Technical Status -- LBL TOUGH2 Products

- Evaluated Parallelizing TOUGHREACT
  - Could take significant effort and resources
  - Question on necessary skill set available in SIGMA^3
  - Software development/modification is not originally scoped in this project
  - Able to compile and run sample problems on TOUGHREACT and TOUGH2v2

Summary – Key Findings/Conclusions

- Lack of a functional Commercially available fully coupled reactive transport simulator is an obstacle in moving forward on this project
- Evaluating, incorporating, and modifying (parallelizing) LBL TOUGHREACT is not part of scope of this project and would take additional resources and funding

Summary – Future Plans

- Evaluate the use of REVEAL reservoir simulator
  - with water chemistry
  - Each cell forced to equilibrium e.g. CSTR (PHREEQC) not a true reactive transport process
- Utilize 3-D layer cake model non-parallelized TOUGHREACT on single node and reduce scope on ED/RSM evaluation
- Evaluate other change of scope opportunities
  - Re-scope and try to work with Universities or consultants to Parallelize TOUGHREACT

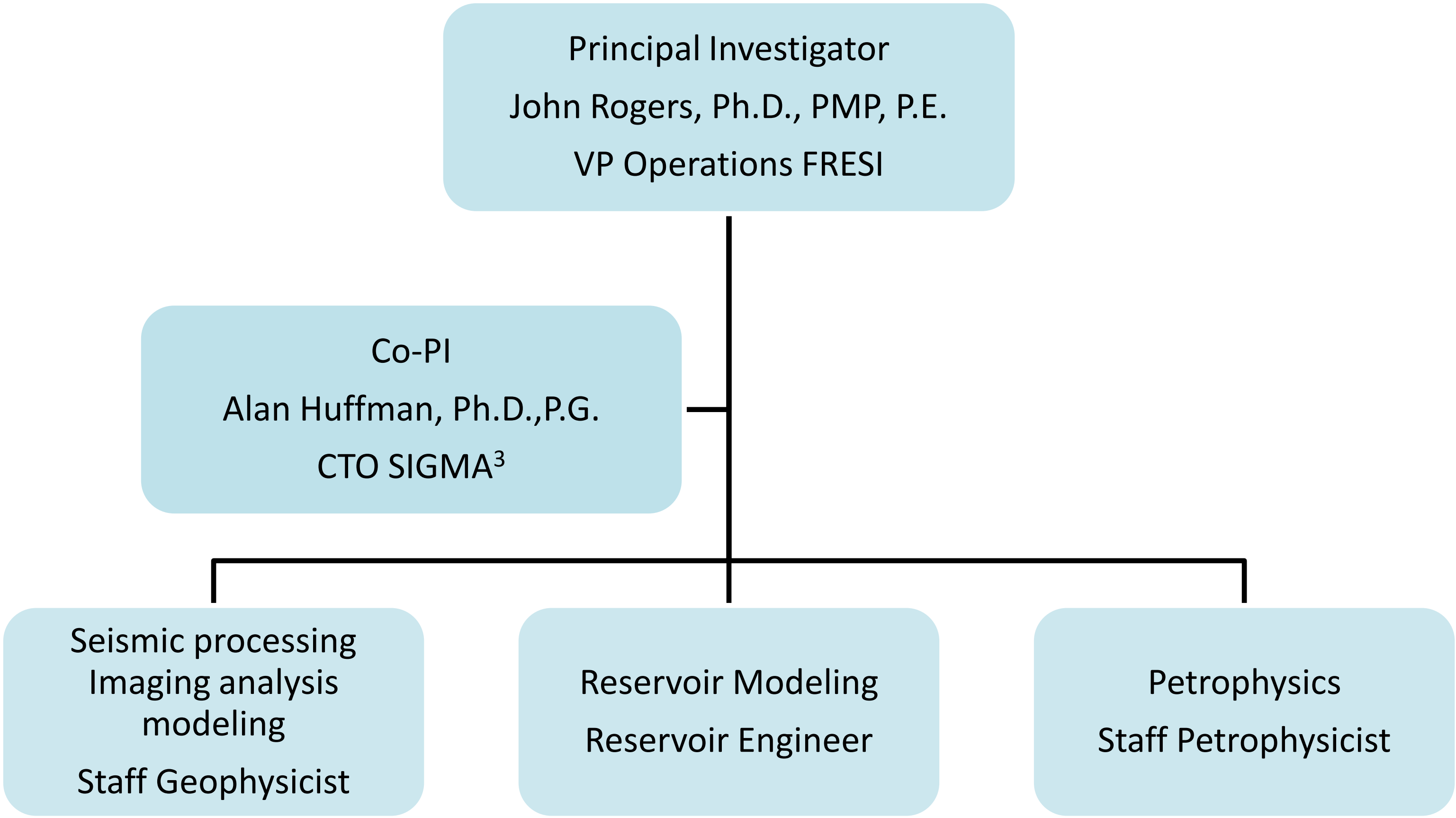
Accomplishments

- Baseline Reservoir Model Defined
- Detailed reservoir characterization model defined
- Detailed Rock mineralogy/assemblage defined
- Commercial third party reactive transport simulator tested

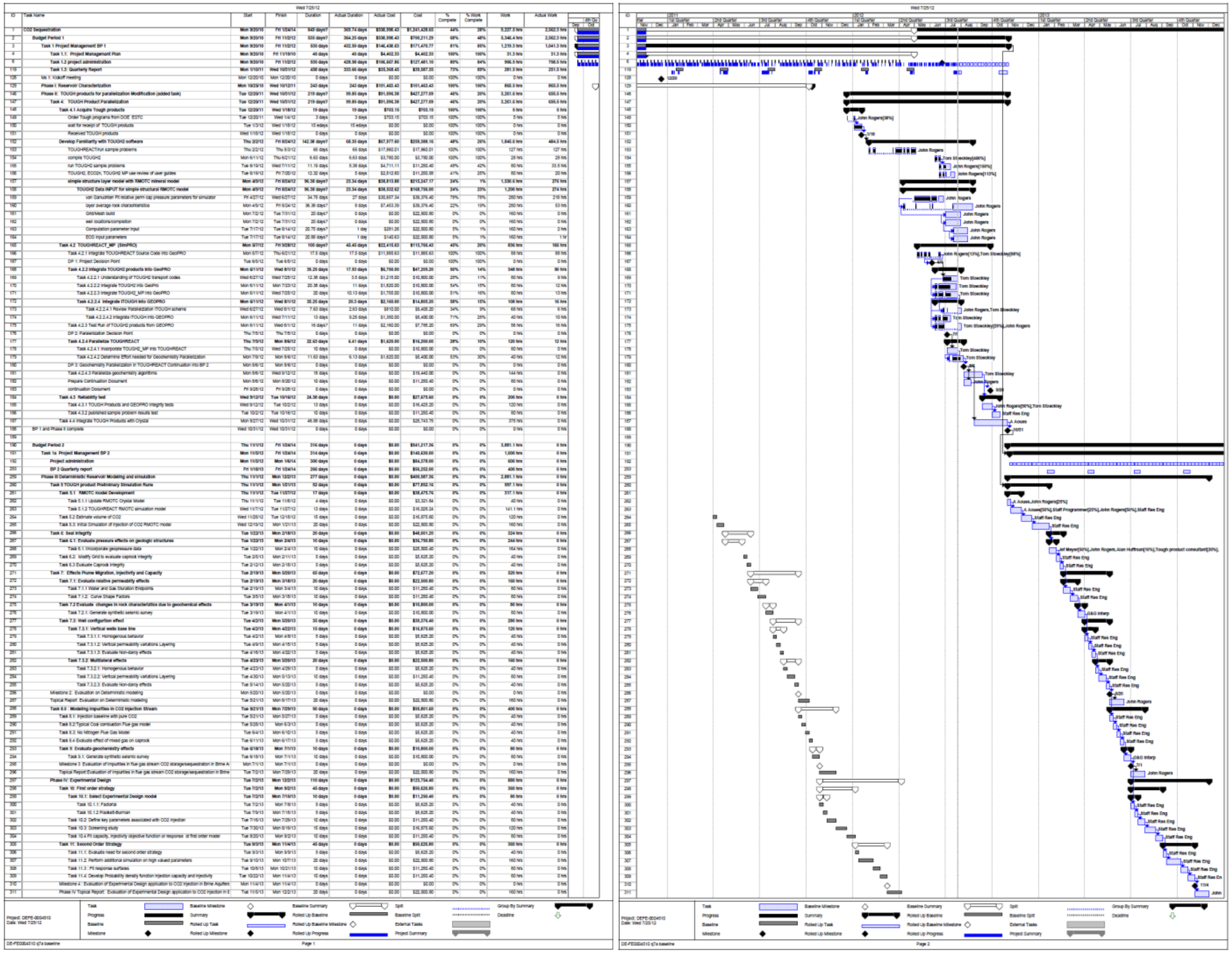
END

APPENDIX

Organization Chart



Gantt Chart



Project Summary

Goals

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

Performance Period

- Three phases in two budget periods; Sep 20, 2010; 19 months
- BP1 Extended to October 31, 2012

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

Status/accomplishments

- Still in BP 1
- Project re-scoping