Sim-SEQ: A Model Comparison Initiative for Geologic Carbon Sequestration

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Developing the Technologies and Building the Infrastructure for CO_2 Storage

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- Jun Li and Lingli Wei (Shell, China)
- Hajime Yamamoto (Taisei Corporation, Japan)
- Yi Zhang (RITE, Japan)
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Presentation Outline

- Project objectives and benefits
- Model uncertainty and the need for a model comparison study for GCS systems
- An overview of the Sim-SEQ project
- Brief Introduction to the Sim-SEQ Study Site
- Selected preliminary conceptual models and model predictions
- Comparison of preliminary model results
- Summary of accomplishments and future steps

Benefit to the Program

The Sim-SEQ project addresses the following goal of the Carbon Storage Program

—Develop technology to demonstrate that 99% of the injected CO_2 remains in the injection zone

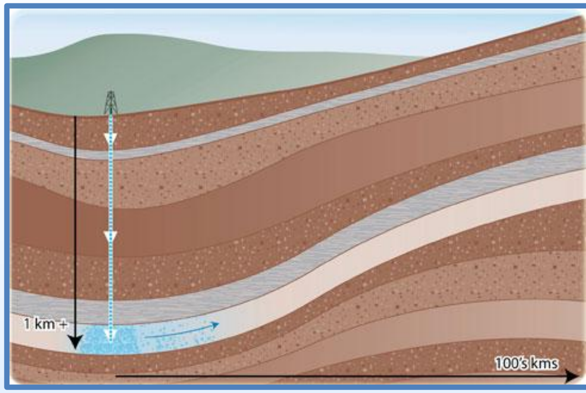
Sim-SEQ is a model comparison initiative with the objective to understand and quantify uncertainties arising from model choices made by modelers.

—It intends to demonstrate in an objective manner that the observed system behavior at GCS sites can be predicted with confidence, and that the remaining differences between models and measurements, as well as between different models, are well understood.

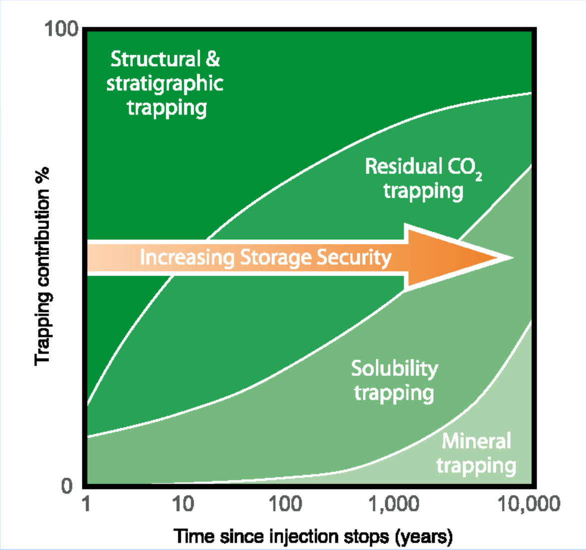
—It ensures that model uncertainties are evaluated and their impact is assessed, and that lessons l earned and improvements are documented and made available to all research teams

Sources of Model Uncertainty

- Need to predict the fate of injected CO_2
- Uncertainty of subsurface processes and of their spatial/temporal scales
- Uncertainty of the subsurface geology and of the distribution of parameters (flow, PVT, geochemistry, etc.)
- Choices made by modelers: software to be used, which processes, coupling of processes, multiple length scales and grid discretization, boundary conditions
- These choices cause a wide range in model predictions



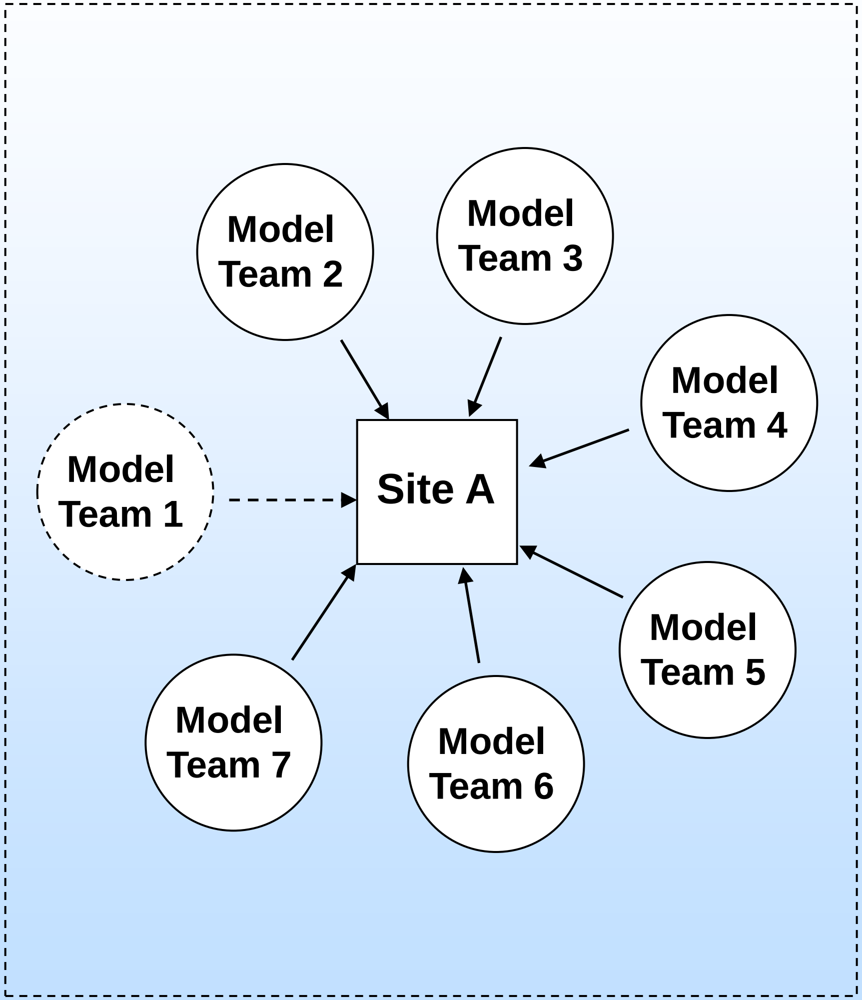
www.co2crc.com.au



Model Comparison

To increase stakeholders' confidence in GCS systems, we need to understand the root causes of model uncertainties and, if possible, quantify these uncertainties

This can be accomplished by engaging in a model comparison study involving both model-to-data and model-to-model comparison at one or more selected GCS field sites.



Sim-SEQ is not Code Comparison or Benchmarking

Benchmarking exercises related to GCS problems have been conducted in the past (Pruess et al., 2004; Class et al., 2009)

In both studies, modelers were provided with precise descriptions of model domains, boundary conditions, rock properties, etc.,

Modelers used a variety of simulators but the same set of input data

Differences in model results were moderate once data interpretation issues had been resolved, and were mostly related to differences in spatial and temporal discretization (Class et al., 2009)

Sim-SEQ is Model Comparison

•Model comparison evaluates modeling studies in a much broader and comprehensive sense.

•Model building comprises all work flow stages - interpretation of site characterization efforts, parameter choices based on measurements, conceptual model choices, spatial variability characteristics, decisions about domain sizes and boundary conditions, etc.

•The DECOVALEX project on model comparison, conducted by several international organizations involved in geologic disposal of nuclear wastes (Tsang et al., 2009) serves as an analog for Sim-SEQ.

Project Overview

•Led and coordinated by Lawrence Berkeley National Laboratory and funded by DOE/NETL

•Patterned on a Phase III SECARB site (Sim-SEQ Study Site or S3 site) – managed by BEG (University of Texas, Austin)

• Fifteen modeling teams and about thirty five modelers are engaged in the model comparison effort

•Teams are building their own conceptual models using the site characterization data given to them

•Projections made by teams are to be compared with each other and to actual measurements

•Spread of projections is a measure of the conceptual model / model selection uncertainty

Sim-SEQ Timeline

- In the works since 2009
- Actual kick-off meeting in April 2011
- After a modest start, currently 15 participating teams
- At the kick-off meeting, the Sim-SEQ web portal was launched (https://gs3.pnl.gov/simseq/wiki) - password protected site, access to Sim-SEQ participants only
- First phase (predictive simulations) is nearing completion (end of FY12); Next phase (model refinement using observation data has also started (Q4 of FY12)

Modeling Teams and Software

No.	Organization/Institution	Name of Software/Model	Further Information
1.	Bureau of Economic Geology, USA	CMG-GEM	http://www.cmgl.ca/software/gem.html
2.	Bureau de Recherches Géologiques et Minières, France	TOUGH2/Eclipse/Petrel	http://esd.lbl.gov/research/projects/tough/software/tough2.htm; http://www.slb.com/services/software/reseng/compositional.aspx; http://www.slb.com/services/software/geo/petrel.aspx
3.	Geological Storage Consultants, USA	VESA	Gasda et al. (2009)
4.	Imperial College, UK	Eclipse	http://www.slb.com/services/software/reseng/compositional.aspx
5.	Institute of Crustal Dynamics, China	CCS_MULTIF	Yang et al. (2011a,b), Yang et al. (2012)
6.	Lawrence Berkeley National Laboratory, USA	TOUGH2-EOS7C	http://esd.lbl.gov/research/projects/tough/software/tough2.html; Pruess and Spycher (2007)
7.	Pacific Northwest National Laboratory	STOMP-CO2E	http://stomp.pnnl.gov; White and Oostrum (2006)
8.	Research Institute of Innovative Technology for the Earth, Japan	TOUGH2-ECO2N	http://esd.lbl.gov/research/projects/tough/software/tough2.html; Pruess and Spycher (2007)
9.	Sandia National Laboratory, USA	Not available	
10.	UFZ, Germany	OpenGeoSys	http://www.ufz.de/export/data/1/19757_OGS_5_concept_V1.pdf
11.	Shell, China	MoReS	Wei (2012)
12.	Taisei Corporation, Japan	TOUGH2-MP/ECO2N	http://esd.lbl.gov/research/projects/tough/
13.	Uni Research, Norway	VESA	Gasda et al. (2009)
14.	University of Stuttgart, Germany	DUMUX	http://www.dumux.org
15.	University of Utah, USA	STOMP-CO2E	http://stomp.pnnl.gov

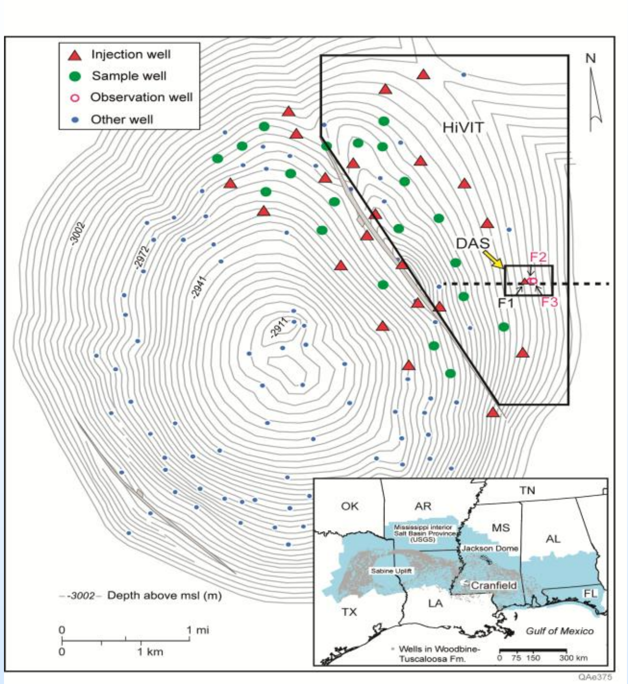
The S-3 Site

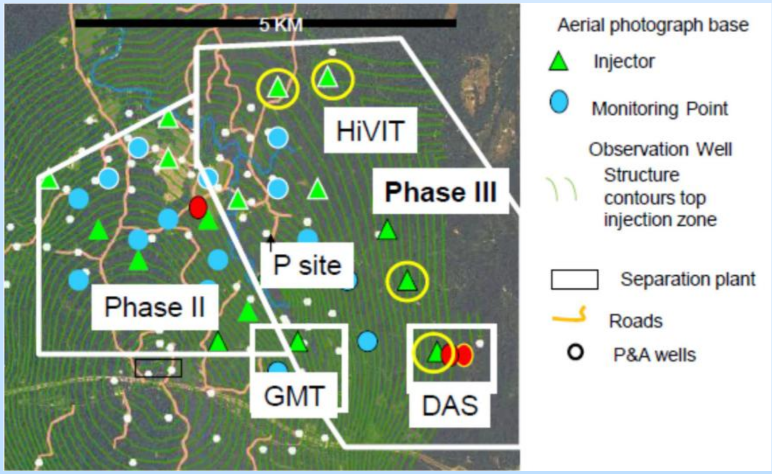
The S-3 site is patterned after the Southeast Regional Carbon Sequestration Partnership (SECARB) Phase III Early Test in the southwestern part of the state of Mississippi in the USA.

The target formation at the S-3 site is comprised of fluvial sandstones of the Cretaceous lower Tuscaloosa Formation at depths of 3300 m

Denbury Onshore LLC has hosted (since 2007) the SECARB Phase II and Phase III tests in a depleted oil and gas reservoir under CO_2 flood.

The tests are managed by the Bureau of Economic Geology (BEG) at the University of Texas, Austin.





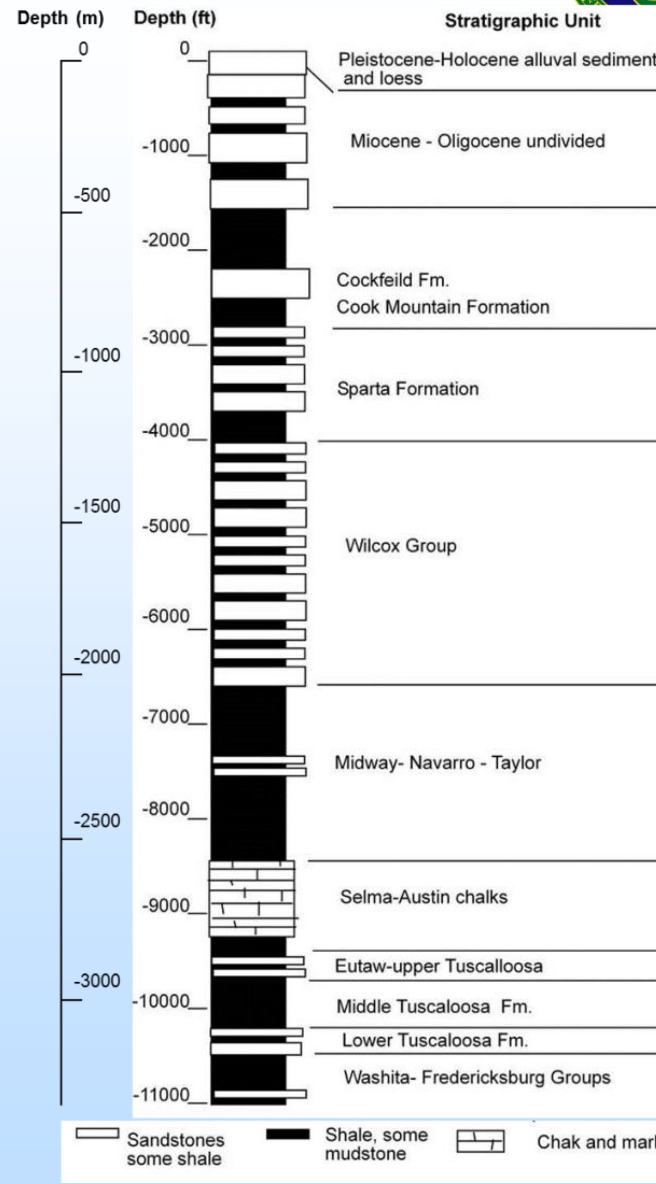
Pictures: Courtesy of JP Nicot (BEG)

Modeling Challenges

The DAS area comprises fluvial deposits of considerable heterogeneity located in the water leg of an active CO_2-EOR field with a strong water drive.

These features add significant complexity when approximating the natural system, and challenges arise in dealing with boundary conditions.

In addition, presence of methane has been confirmed in the brine, which can potentially exsolve and impact pressure buildup history and CO_2 plume extent



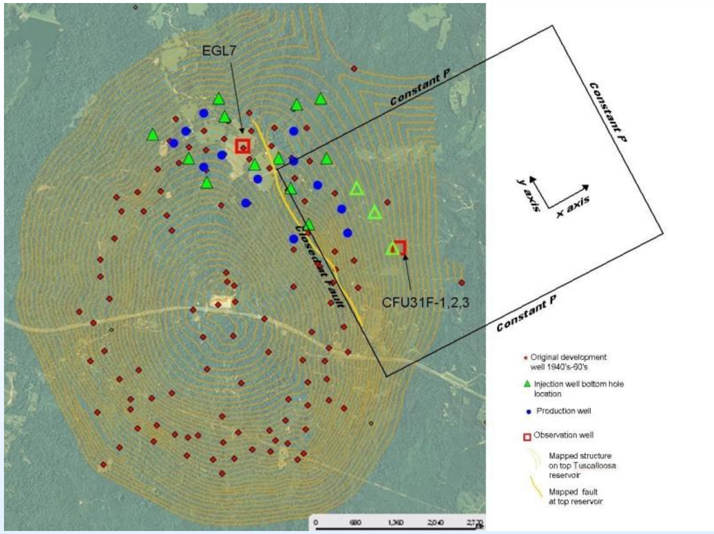
Acknowledgment: JP Nicot (BEG)

Preliminary Conceptual Models of the S-3 Site

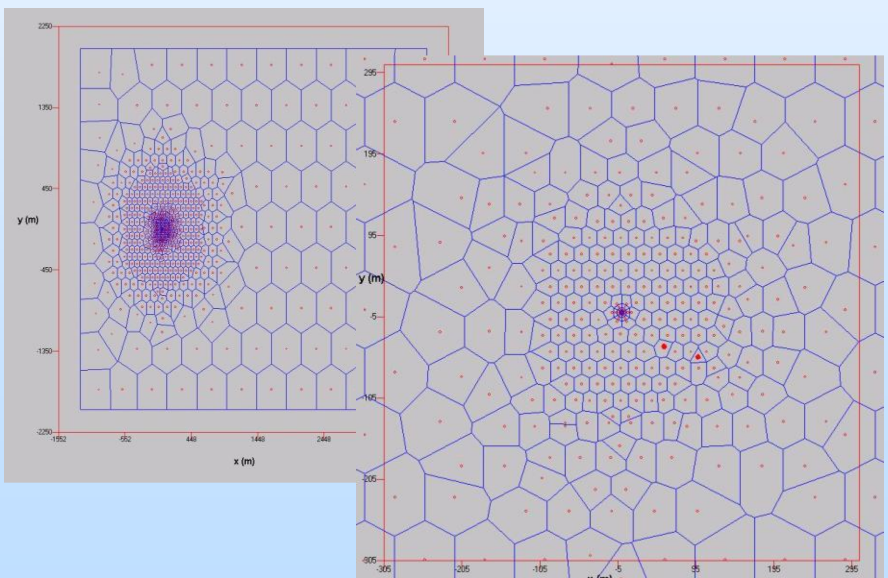
- Eight teams have so far submitted preliminary model results along with the attributes of their conceptual models
  1. PNNL
  2. CIPR, Uni Research, Norway
  3. BRGM, France
  4. Taisei Corporation, Japan
  5. RITE, Japan
  6. Shell, China
  7. Imperial College, London
  8. LBNL

Attributes of the Selected Conceptual Models

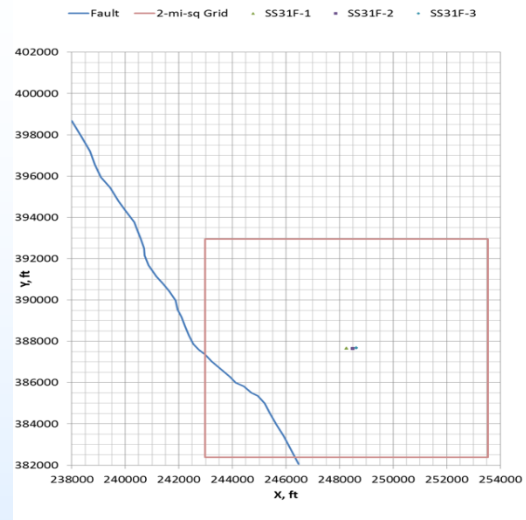
	PNNL	LBNL	Taisei, Japan	Shell, China
Software	STOMP/-WCSE	TOUGH2/EOS7C	TOUGH2/ECO2N	MoReS
Grid Type	3-D, Irregular, Rectangular	3-D Irregular Voronoi Tesselation	Cylindrical, Voronoi Tesselation	3-D, Rectangular
Grid orientation	Boundary-fitted	Tilted	N/A	Tilted
Horizontal model extent	2 mile square	4,000 m × 5,200 m	1,200 m radial centered on F-1	5,000 m × 5,000 m
Vertical layers	16	8	50	40



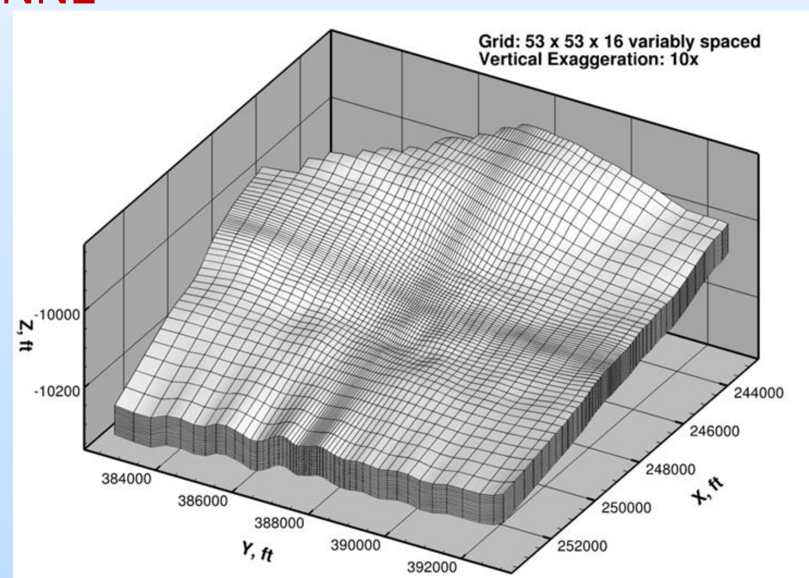
LBNL



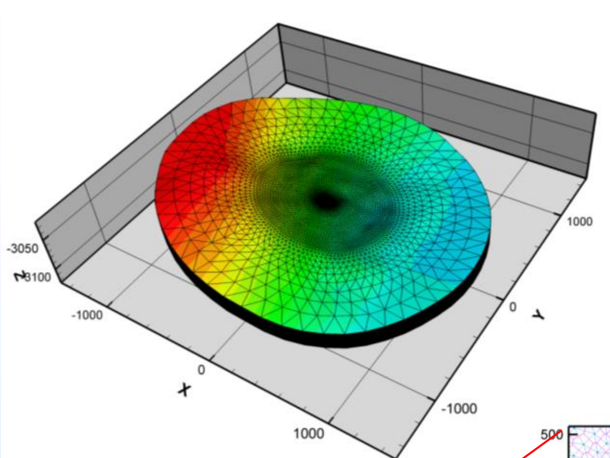
Total Gridblocks: 4,968



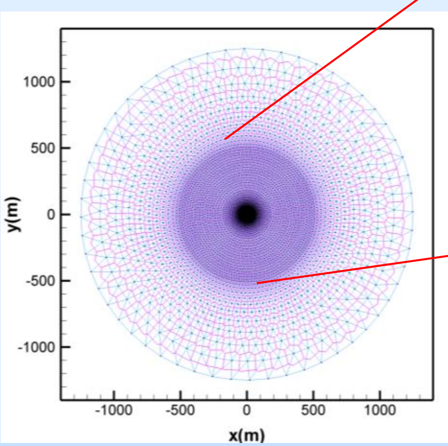
PNNL

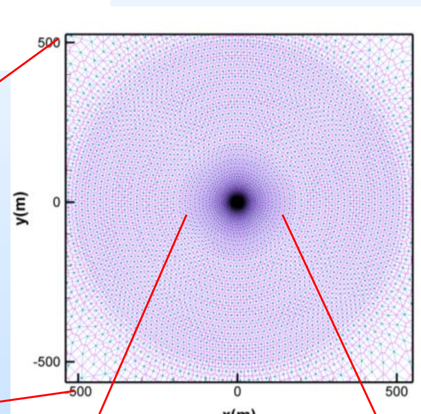


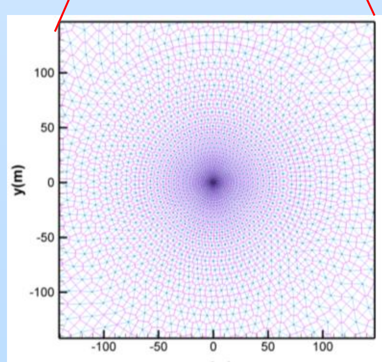
Total Gridblocks: 44,944



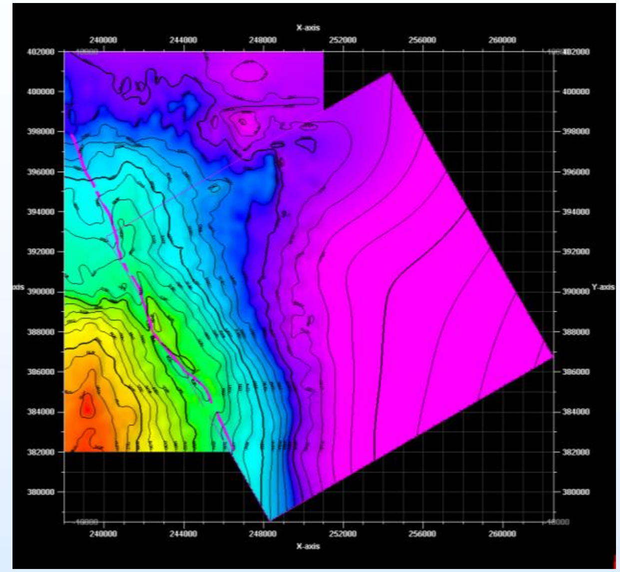
Taisei, Japan

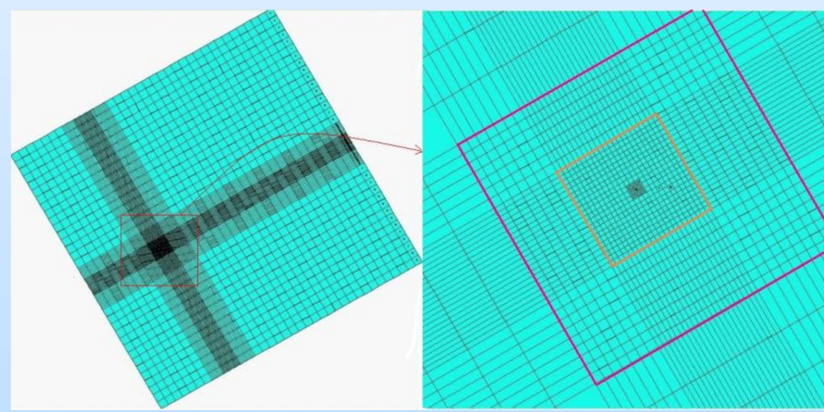






Gridblocks = 223901
Connections = 887,915
(4478 x 50 layers + 1 well)





Total gridblocks: 67x68x40 = 182,240

Shell, China

Boundary and Initial Conditions

	PNNL	LBNL	Taisei, Japan	Shell, China
Fault	No flow	No flow	Not considered	No flow
Top/bottom boundaries	Closed to flow	Closed to flow	Closed to flow	Closed to flow
Side boundaries	Constant pressure	Constant pressure	Constant pressure	Semi-analytical aquifer model or closed
Initial pressure	~32 MPa	~32 MPa	~32 MPa	~32 MPa
Initial temperature	128^{o}C	127^{o}C	100^{o}C	128^{o}C
Initial salt	0.157 ppm	Salt not included	0.123 ppm	0.150 ppm
CH_4	Not included	Water saturated with dissolved CH_4	Not included	Not included

Rock Properties

	PNNL	LBNL	Taisei, Japan	Shell, China
Permeability /porosity	Heterogeneous	Homogeneous (layerwise)	Homogeneous (layerwise)	Heterogeneous
Source of permeability and porosity data	Core data from the two observation wells	Well logs and sidewall cores from the injection well	Log data from observation well F3	Core data from the two observation wells
Permeability anisotropy	Yes	Yes	No	Yes
Permeability upscaling	Yes	Yes	Not	Yes
Relative permeability	Fitted to core measurements	Generic – Corey-like	van Genuchten	Corey
Capillary pressure	Brooks & Corey	van Genuchten	van Genuchten	Fitted to core samples
Residual gas saturation	0.20 (maximum)	0	0	0 and 0.2

PNNL Transition Probability Based Facies Model

Facies 1: Standstone (orange)

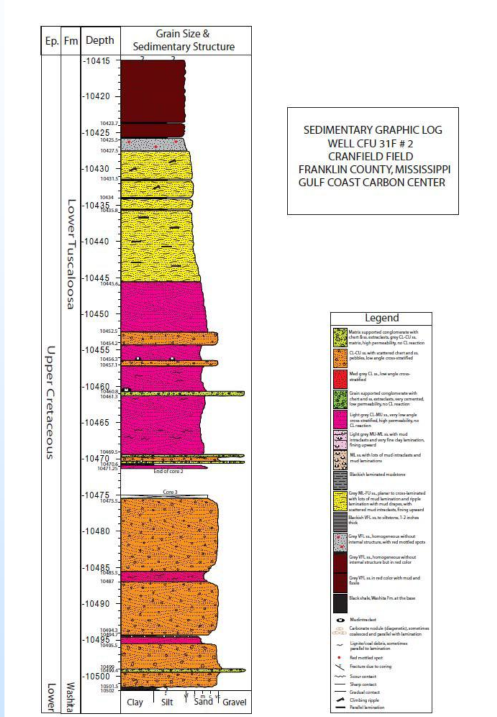
Mean perm: 359.68 mD
Variance: 3.39
Porosity: 0.27

Facies 2: Sandstone and conglomerate (hot pink)

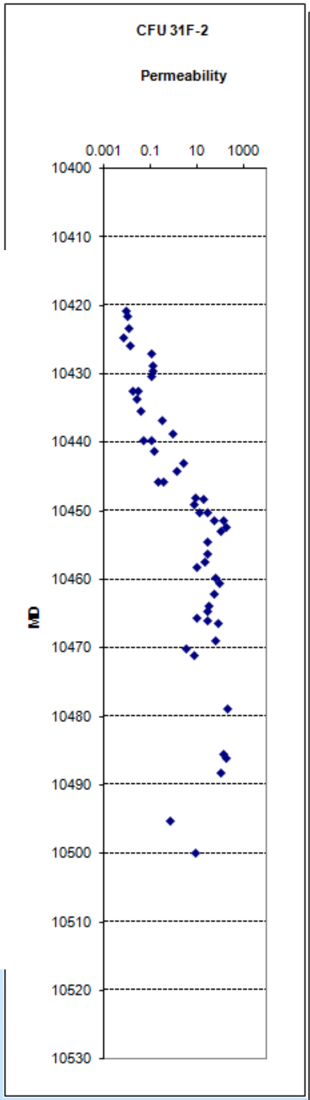
Mean perm: 44.25 mD
Variance: 2.21
Porosity: 0.26

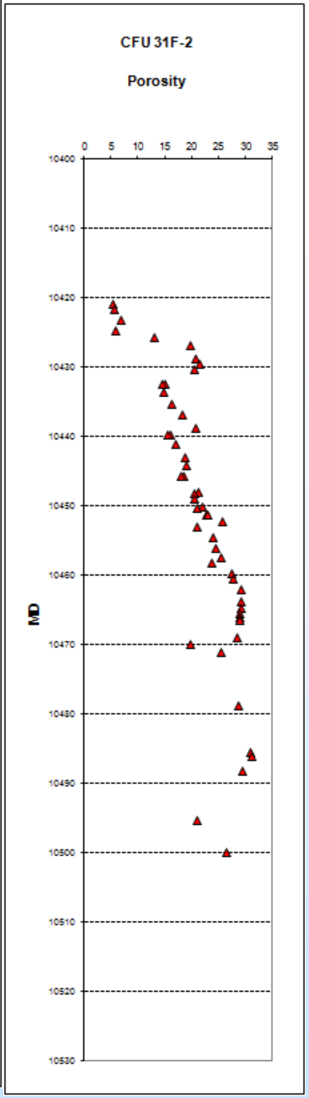
Facies 3: Everything else

Mean perm: 9.07 mD
Variance: 6.63
Porosity: 0.16



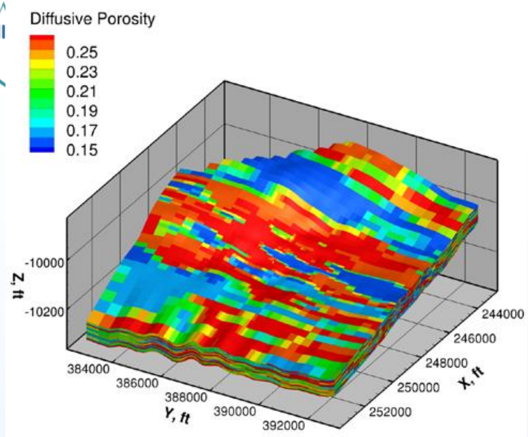
Petrographic Analysis from F2



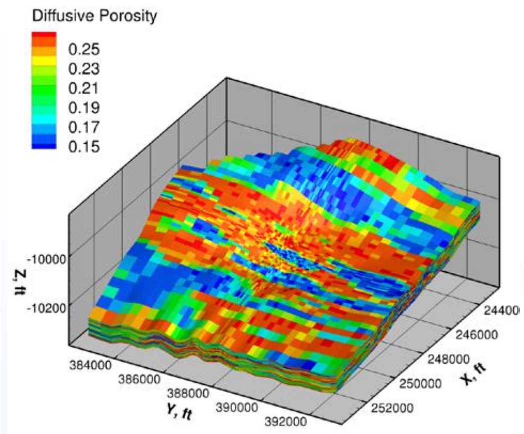


Observation Wells F2 and F3 Core Data
Porosity : 1.29-31.44%; mean 21.76%
Permeability: 0.01-1890 mD; mean: 2.91 mD

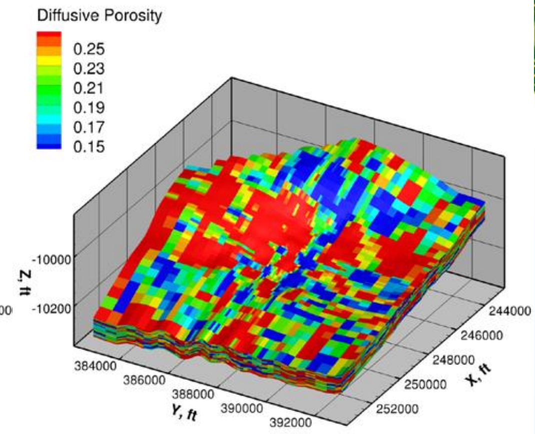
PNNL



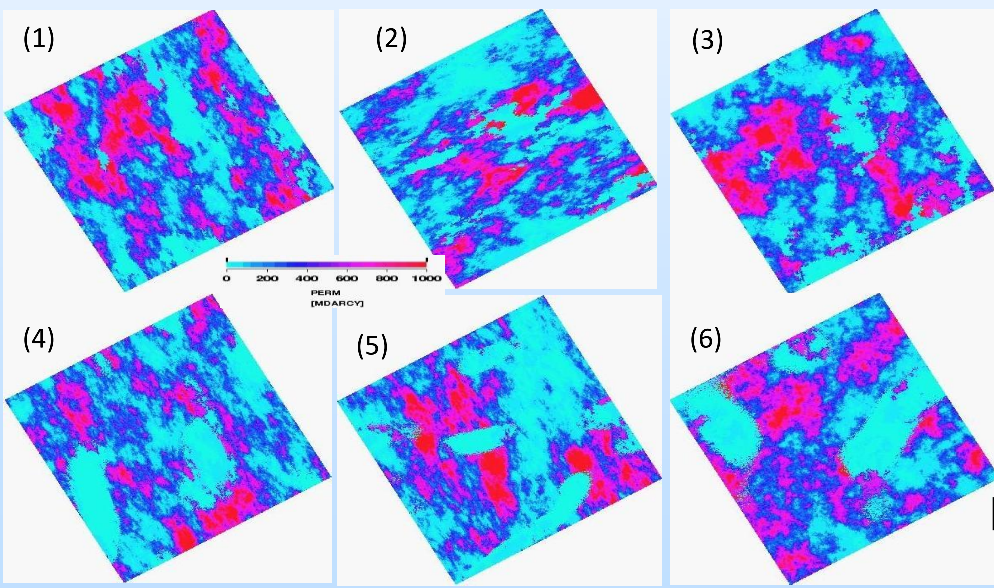
Realization #1 (perm/poro constant in each facies)



Realization #4 (perm/poro random in each facies)



Realization #7 (perm/poro Gaussian in each facies)



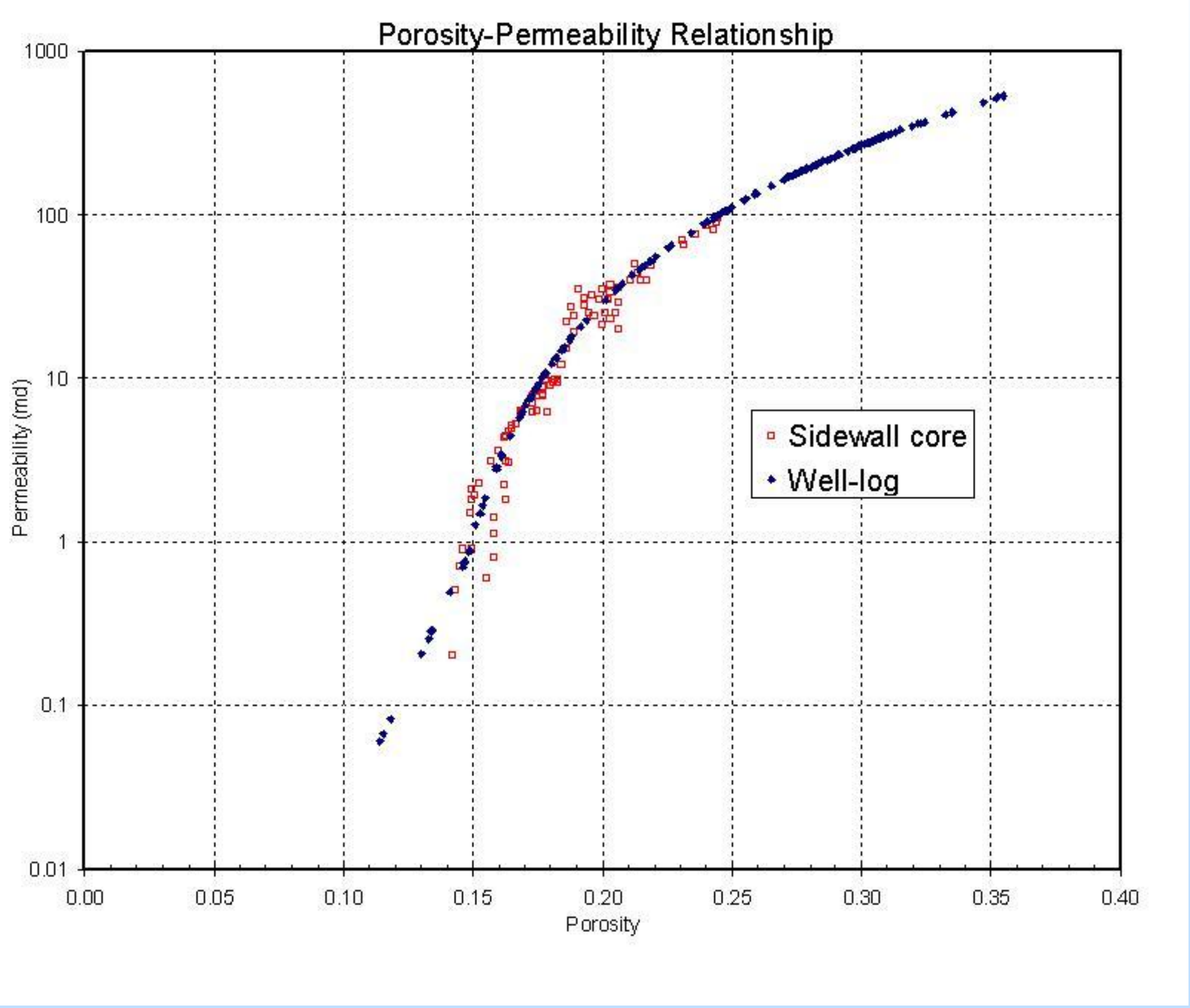
	Anisotropy (2:1)	Anisotropy (1:2)	Anisotropy (1:1)
Sequential indicator	GeoModel1	GeoModel2	GeoModel3
Truncation Gaussian	GeoModel4	GeoModel5	GeoModel6

Permeability scale 0 (cyan)-400 mD (red)

Shell, China

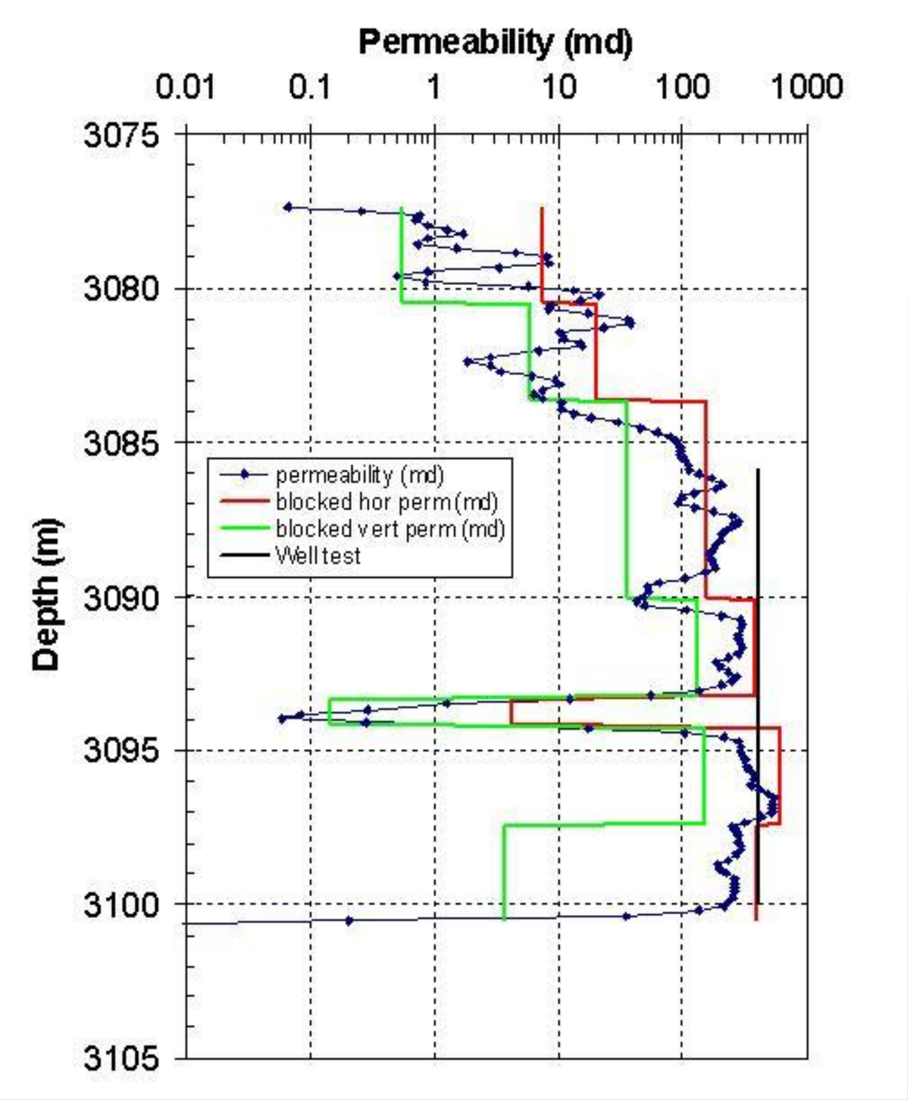
Well-log Data

- Well log includes
  - SP
  - gamma
  - density porosity
  - VP
- Sidewall core includes porosity and permeability for a subset of depths – high porosity values missing
- Use sidewall core to develop a porosity-permeability relationship and extrapolate to entire porosity range

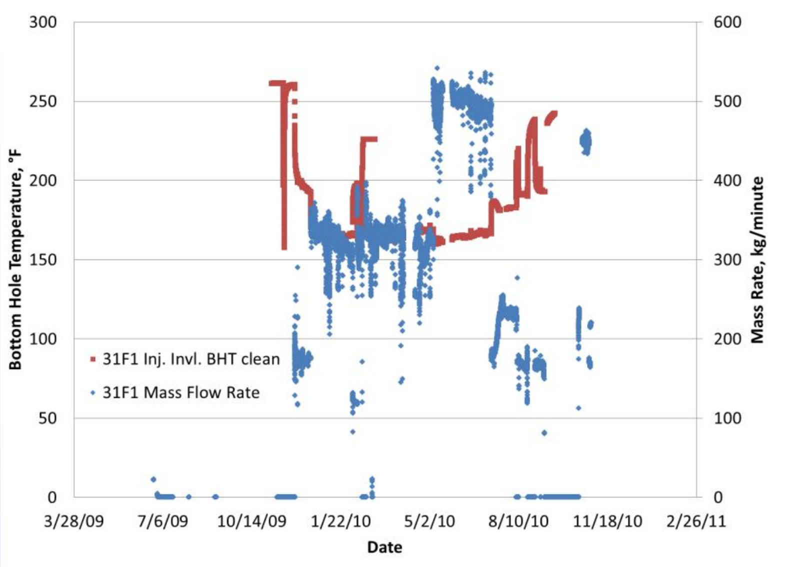


LBNL Layer Properties

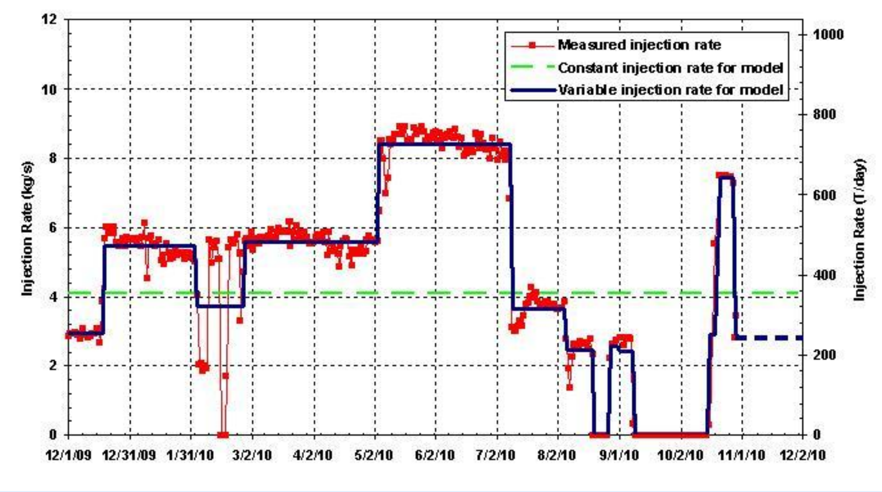
- Layers are equal thickness except for one thinner low-permeability layer inferred to be a shale baffle
- Well-log permeabilities are scaled to well-test permeability (multiply by 1.76)
- Arithmetic average for horizontal permeability
- Harmonic average for vertical permeability, times anisotropy factor of 0.5 (literature value)
- No lateral heterogeneity, except well column permeability decreased to represent skin effect (well-test analysis)



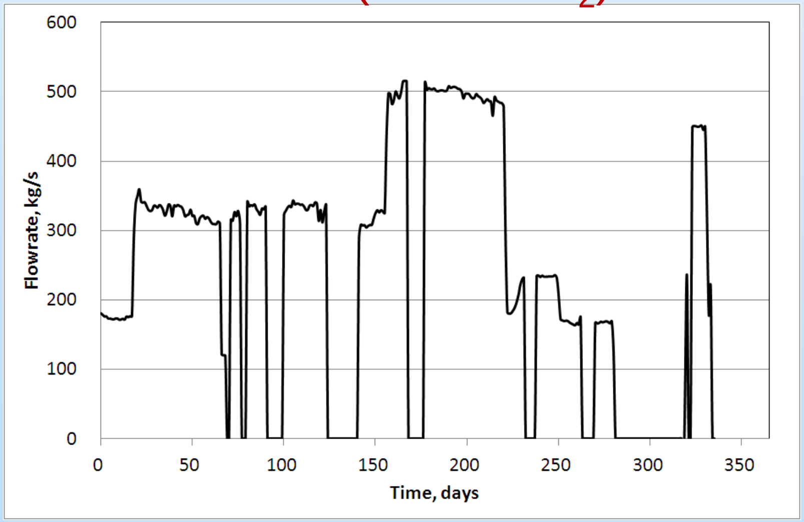
Injection Rate



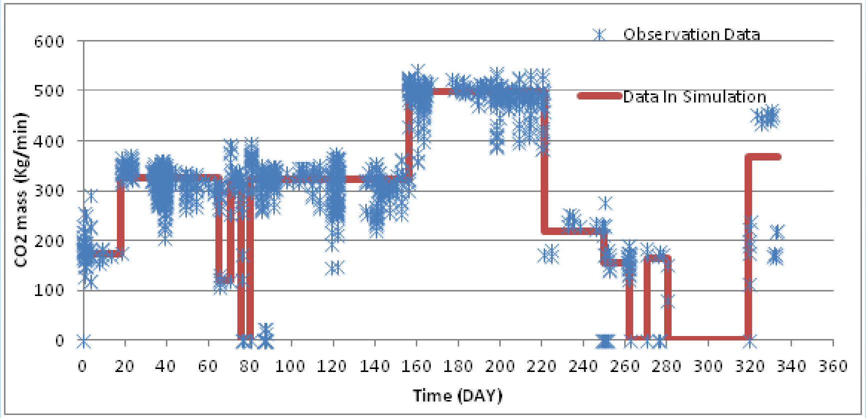
PNNL (100% CO_2)



LBNL (92% CO_2, 8% CH_4)

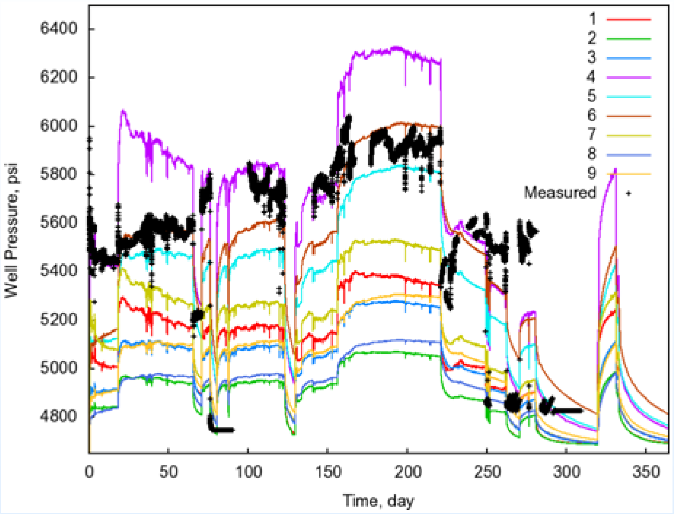


Taisei, Japan (100% CO_2)

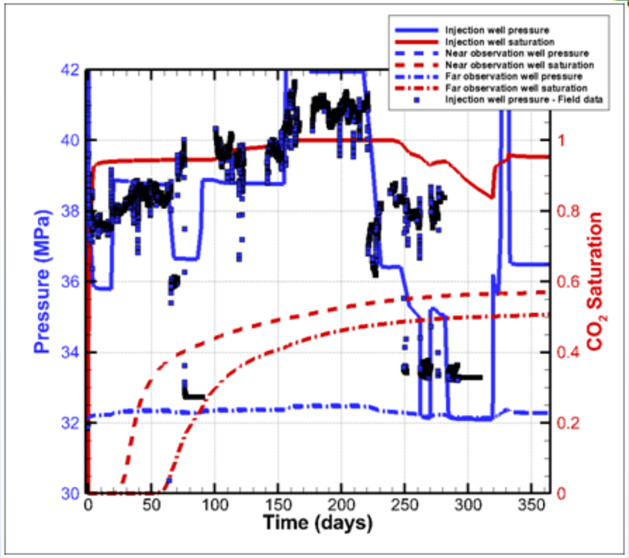


Shell, China (100% CO_2)

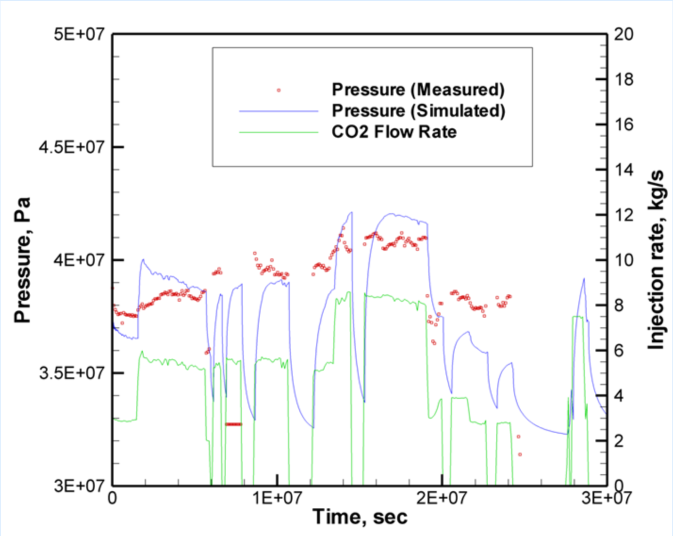
Simulated Vs. Observed Bottomhole Pressure



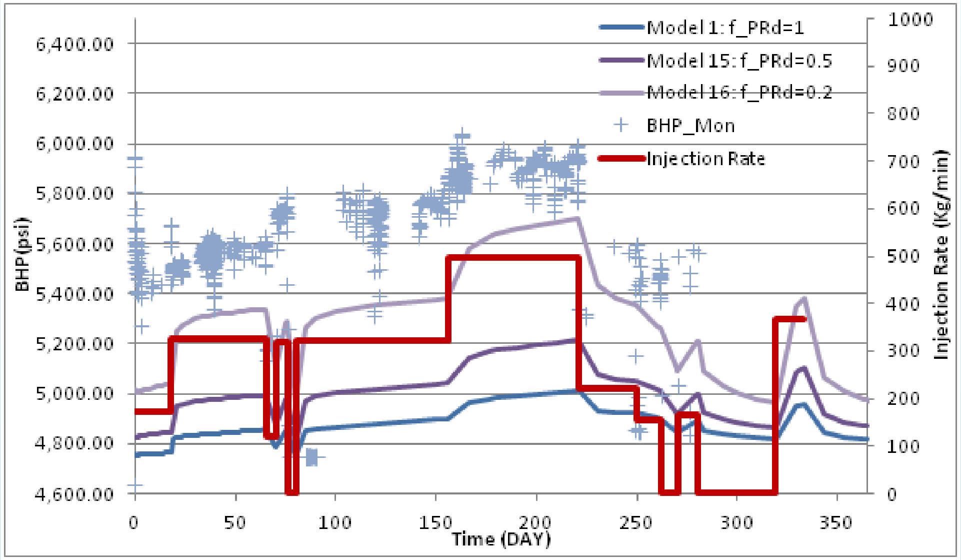
PNNL



LBNL

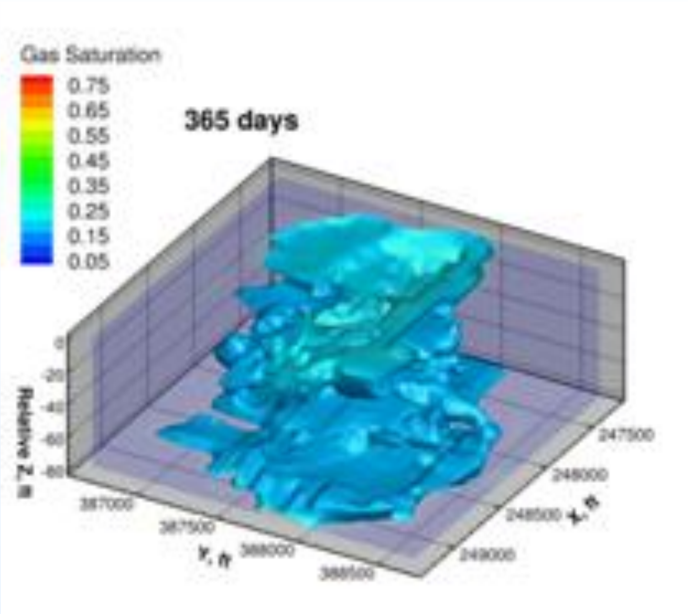


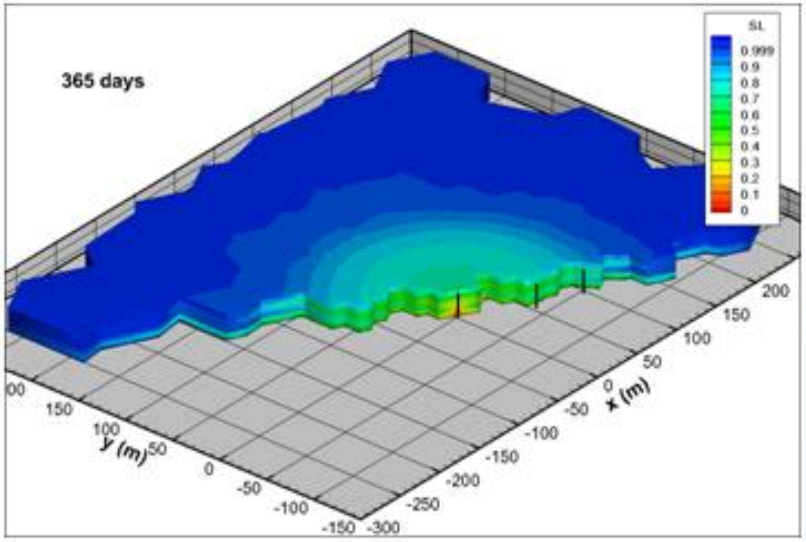
Taisei, Japan



Shell, China

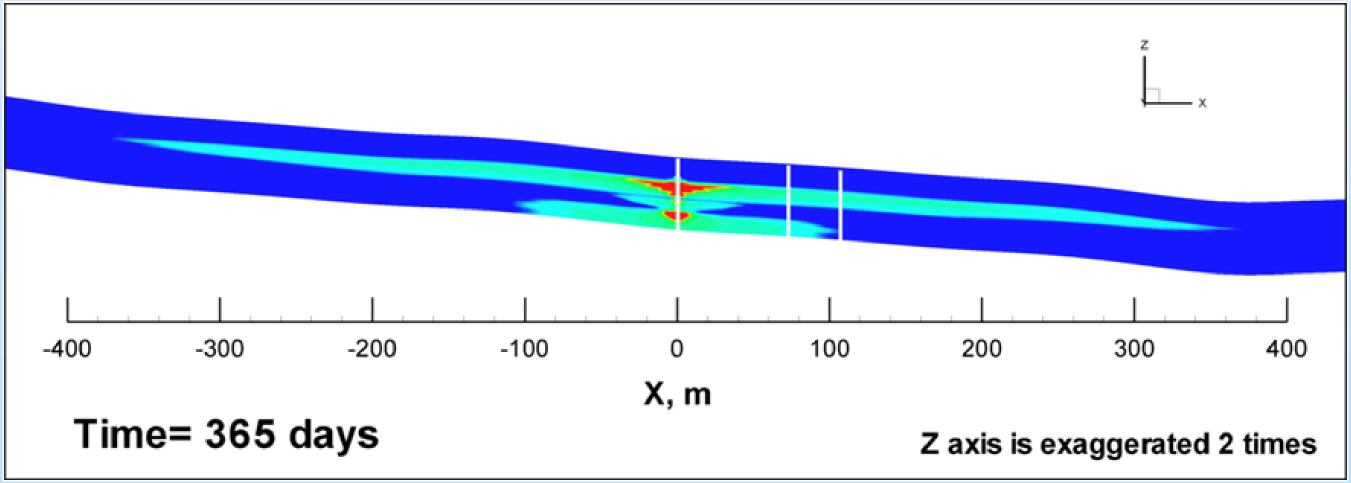
Contours of Supercritical CO_2 at 1 Year





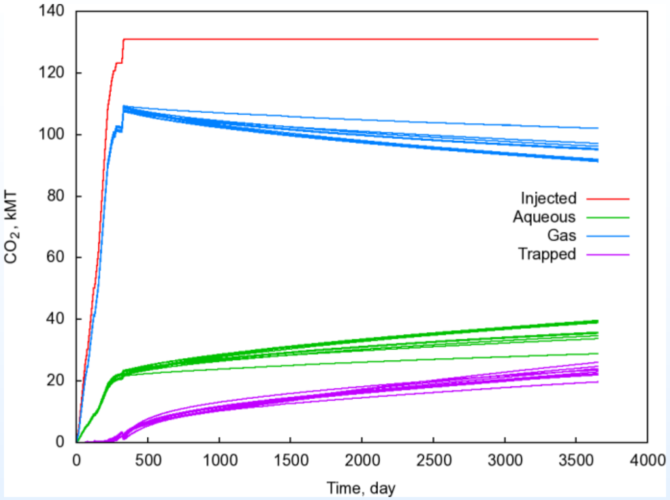
LBNL

PNNL

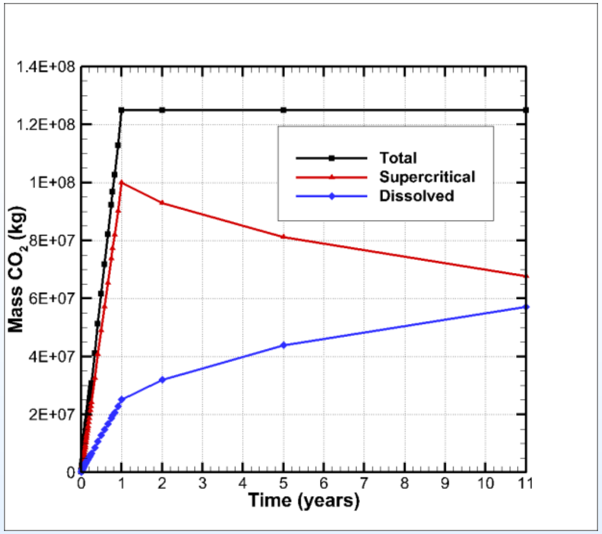


Taisei, Japan

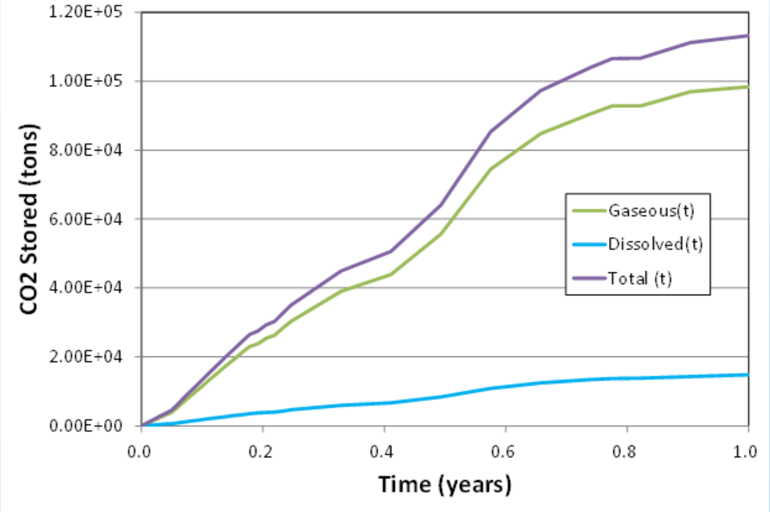
Phase Distribution of Injected CO_2



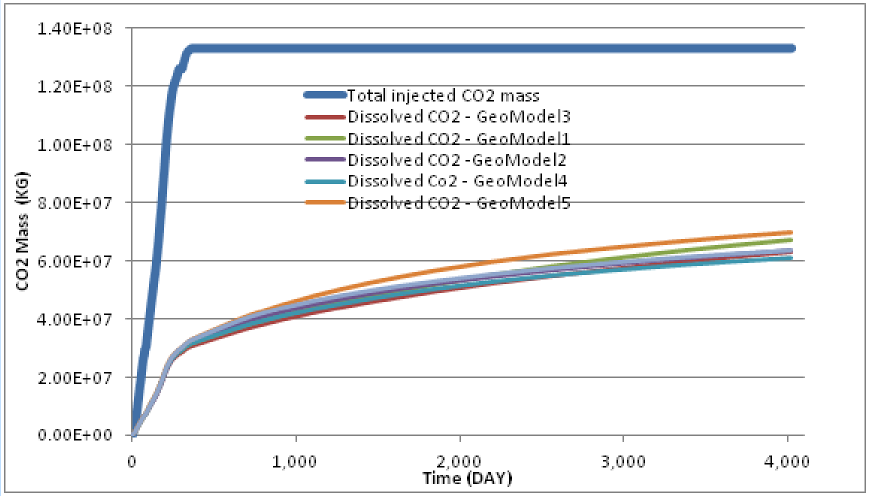
PNNL



LBNL



Taisei, Japan



Shell, China

Comparison of Preliminary Model Results

Acknowledgment: JP Nicot (BEG)

Model	% CO_2 in Gas Phase at 1 year	CO_2 Arrival Time at Well F2 (Days)	CO_2 Arrival Time at Well F3 (Days)
PNNL	84	8-14	19-53
LBNL	79	19	53
Taisei, Japan	87	9	22
Shell, China	76	16-22	30-48
BRGM, France	89	11	34
RITE, Japan	85	12	18
CIPR, Norway	95	27	65
Imperial College, London	86	36	94

<u>Range of Prediction</u>

CO_2 in Gas Phase: 76-95%
Arrival Time at F2: 8-36 days
Arrival Time at F3: 18-94 days

Differences in model conceptualization cause a large range in predictions

Key Accomplishments to Date

- ❖An international collaboration involving many modeling teams has been initiated for model comparison in GCS systems
- ❖A website for Sim-SEQ is fully operational
- ❖Preliminary model results have been obtained and qualitative model comparison is in progress – key model attributes for prediction uncertainties are being identified. Performance metrics for model comparison have been established
- ❖An integrated uncertainty quantification framework has been proposed and is currently being evaluated for application in Sim-SEQ
- ❖Multiple workshops, teleconferences and webinars have been organized for dissemination of information among modeling teams

Summary and Future Steps

- To understand the root causes of model uncertainties in GCS systems, Sim-SEQ is engaged in a model-to-model and model-to-data comparison study at one selected field CO_2 injection test site.
- Qualitative comparison of preliminary model results confirms that model choices made by different modelers indeed impact the range of model predictions, even though each of the modeling team is addressing the same injection scenario at the same GCS site.
- Better understanding and representation of the site characterization data in the conceptual models are likely to improve the model predictions
- Future steps include
  - Iterative improvement of the conceptual models utilizing observation data from the S-3 site.
  - Quantitative model comparison and uncertainty analysis
  - Extension of the model comparison effort to other GCS sites

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Appendix

Project Management

PI: Sumit Mukhopadhyay

LBNL: Coordinates the model comparison effort

- Organizes and facilitates video- and teleconferences and workshops
- Performs status review of model plans, including model approaches, schedules, and code capabilities
- Develops modeling performance metrics for comparison of predictions and measurements
- Conducts timely review and evaluation of model results
- Mediates discussion about model improvement and develop list of lessons learned
- Summarizes model comparison results in annual reports

All Model Teams are involved in all the activities listed above

Organization Chart

PI: Sumit Mukhopadhyay (LBNL)

No.	Organization/Institution	Name of Software/Model	Further Information
1.	Bureau of Economic Geology, USA	CMG-GEM	http://www.cmgl.ca/software/gem.html
2.	Bureau de Recherches Géologiques et Minières, France	TOUGH2/Eclipse /Petrel	http://esd.lbl.gov/research/projects/tough/software/tough2.htm; http://www.slb.com/services/software/reseng/compositional.aspx; http://www.slb.com/services/software/geo/petrel.aspx
3.	Geological Storage Consultants, USA	VESA	Gasda et al. (2009)
4.	Imperial College, UK	Eclipse	http://www.slb.com/services/software/reseng/compositional.aspx
5.	Institute of Crustal Dynamics, China	CCS_MULTIF	Yang et al. (2011a,b), Yang et al. (2012)
6.	Lawrence Berkeley National Laboratory, USA	TOUGH2-EOS7C	http://esd.lbl.gov/research/projects/tough/software/tough2.html; Pruess and Spycher (2007)
7.	Pacific Northwest National Laboratory	STOMP-CO2E	http://stomp.pnnl.gov; White and Oostrum (2006)
8.	Research Institute of Innovative Technology for the Earth, Japan	TOUGH2-ECO2N	http://esd.lbl.gov/research/projects/tough/software/tough2.html; Pruess and Spycher (2007)
9.	Sandia National Laboratory, USA	Not available	
10.	UFZ, Germany	OpenGeoSys	http://www.ufz.de/export/data/1/19757_OGS_5_concept_V1.pdf
11.	Shell, China	MoReS	Wei (2012)
12.	Taisei Corporation, Japan	TOUGH2-MP/ECO2N	http://esd.lbl.gov/research/projects/tough/
13.	Uni Research, Norway	VESA	Gasda et al. (2009)
14.	University of Stuttgart, Germany	DUMUX	http://www.dumux.org
15.	University of Utah, USA	STOMP-CO2E	http://stomp.pnnl.gov

Gantt Chart

Year	FY11				FY12				FY13				FY14			
Quarter	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
Task 1: Data Review and Site Selection	-	-	-													
Task 2: Model Development	-	-	-													
Task 3: Predictive Simulations	-	-	-													
Task 4: Model Refinement	-	-	-													
Task 5: Technical Team Participation	-	-	-													
Annual Reports	-	-	-													

Bibliography

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