Web-based CO_2 Subsurface Modeling

Geologic Sequestration Training and Research

Project Number DE-FE0002069

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U.S. Department of Energy

National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and Building the
Infrastructure for CO_2 Storage

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Presentation Outline

- Project benefits and goals.
- Web interface for simulating water-rock interaction.
- Development of, and experience teaching, a new Carbon Capture and Sequestration course at San Diego State University.
- Some noteworthy results of student research and training in CCS oriented geochemistry.
- Status of active student geochemical and geomechancal modeling projects.
- Project accomplishments and summary.

Benefit to the Program

- **Overall program goal:** initiate geologic sequestration training and research at San Diego State University (SDSU)
  - Develop a Rich Internet Application (RIA) interface to a baseline water-rock interaction code developed by Sienna Geodynamics and donated to SDSU to introduce students to CCS.
  - Develop a new cross-disciplinary graduate level class in CCS that uses the RIA with data from existing test sites.
  - Extend baseline code with student developed heat-transfer, poroelastic, and parallel solute mass-transfer modules.
- **Project benefits:** The RIA and extended water-rock interaction code developed through this project directly addresses the need for development of models that include full coupling of geochemical processes (subsurface chemical reactions among CO_2, groundwater/brine, and rock) and geomechanical processes, as specified in the original solicitation, and has lead to an improved ability to numerically model sub-surface CO_2. *This technology contributes to the Carbon Storage Program's effort to develop technologies that will support industries' ability to predict CO_2 storage capacity in geologic formations to within ±30 percent. (Goal).*

Project Overview: Goals and Objectives

- **Statement of Project Objectives** (**SOPO) Goal #1:** create a Web-based simulator with comprehensive chemical and physical numerical processes relevant for modeling CO_2 sequestration scenarios. Success criteria: goal met (Y/N)
- **SOPO Goal #2:** use developed Web-based simulator as part of a new course on CO_2 sequestration and modeling at San Diego State University (SDSU). Goal met (Y/N)

SOPO goals 1 and 2 support the Carbon Storage Program major goal of developing technologies that will support industries' ability to predict CO_2 storage capacity in geologic formations to within ±30 percent

- **SOPO Goal #3:** provide an opportunity at SDSU to further develop existing industry-supported multidisciplinary applied computational science program. Goal met (Y/N)
- **SOPO Goal #4:** provide industry with graduates trained in CCS simulation.

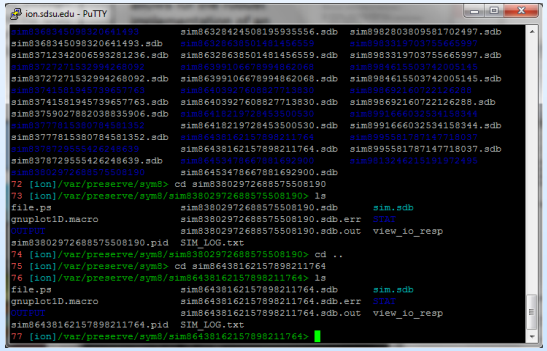
Success criteria: internships and placement of students in CCS programs

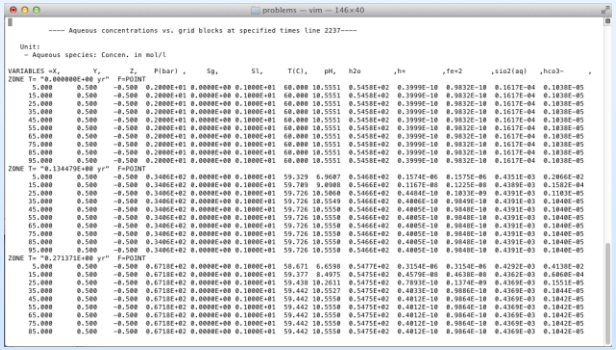
SOPO goals 3 and 4 support the Carbon Storage Program major goals of providing the industry with people who can (1) develop technologies to demonstrate that 99 percent of injected CO_2 remains in the injection zones and (2) conduct field tests through 2030 to support the development of BPMs for site selection, characterization, site operations, and closure practices.

Technical Status

SOPO Goal #1: RIA for Simulating Water-Rock Interaction

- Impetus: steep learning curve for geology and chemistry undergraduates in using command-line, Unix based textual tools such as TOUGHREACT, EQ3/6, and EQ3NR.
- Student experiences with TOUGHREACT: difficult to understand and configure multiple input files, difficulty with post-processing and result visualization (typically with MATLAB).

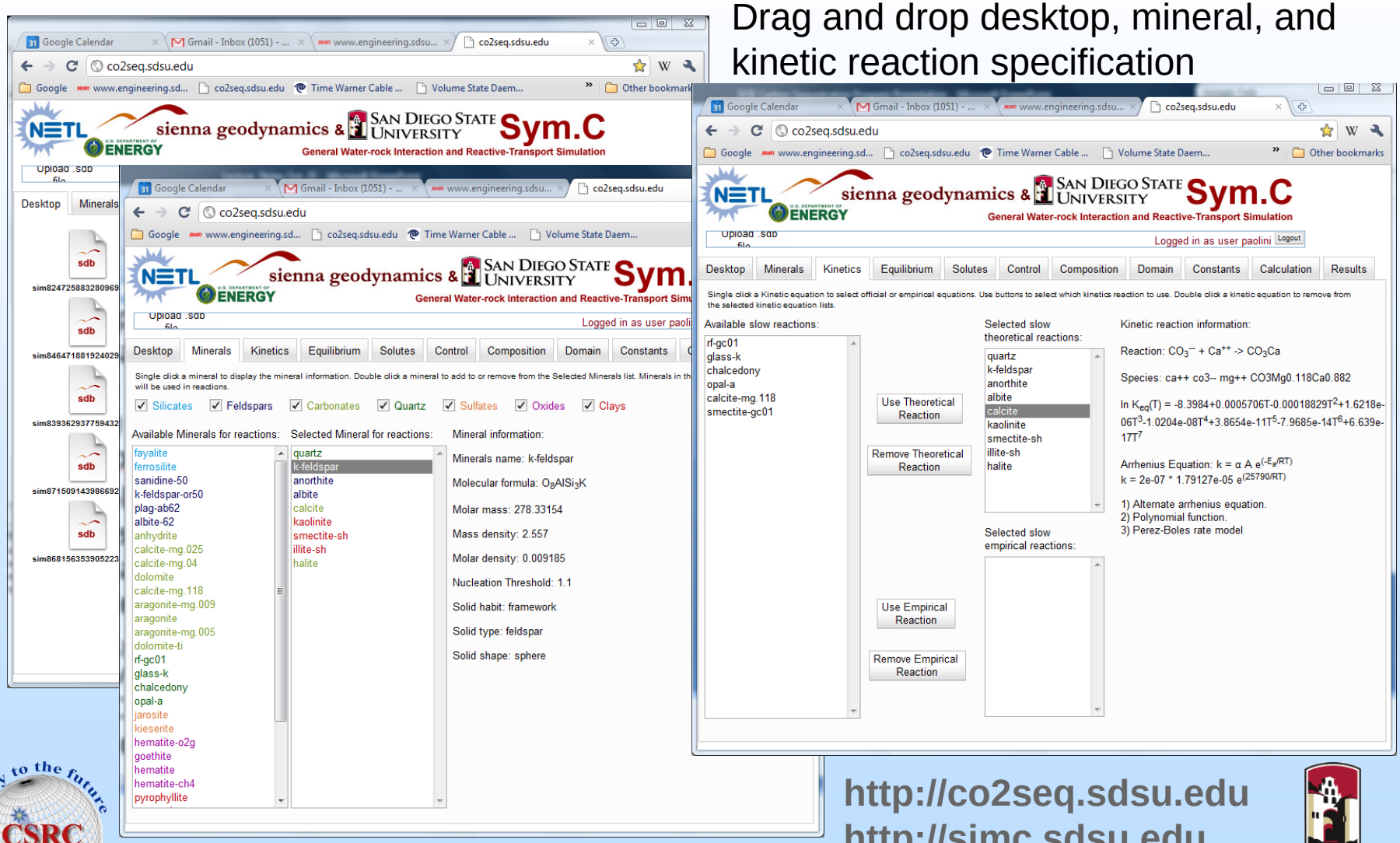




- Idea: develop intuitive Web application that can function as a wrapper around an existing water-rock interaction code that geology and chemistry students, with little or no Unix/Linux skills, can use to model and simulate typical CCS scenarios.
- Selected water-rock interaction code was *Sim.8* from Sienna Geodynamics & Consulting, Inc., through partnership with SDSU.

Technical Status

SOPO Goal #1: RIA for Simulating Water-Rock Interaction



Drag and drop desktop, mineral, and kinetic reaction specification

http://co2seq.sdsu.edu
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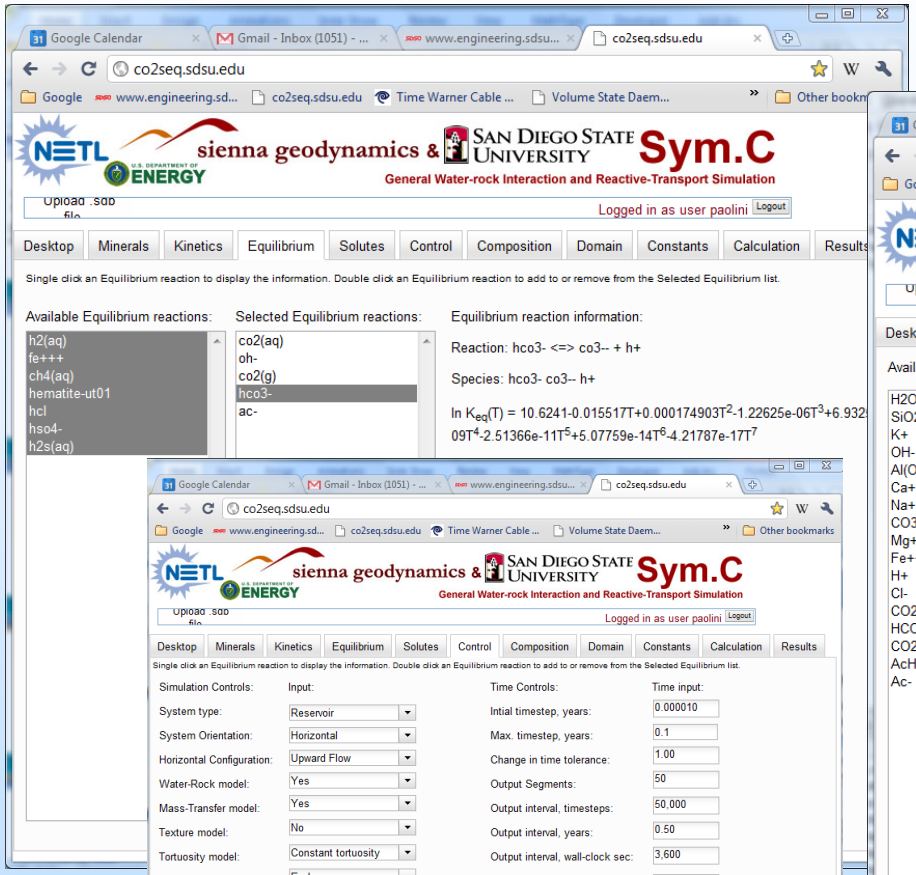
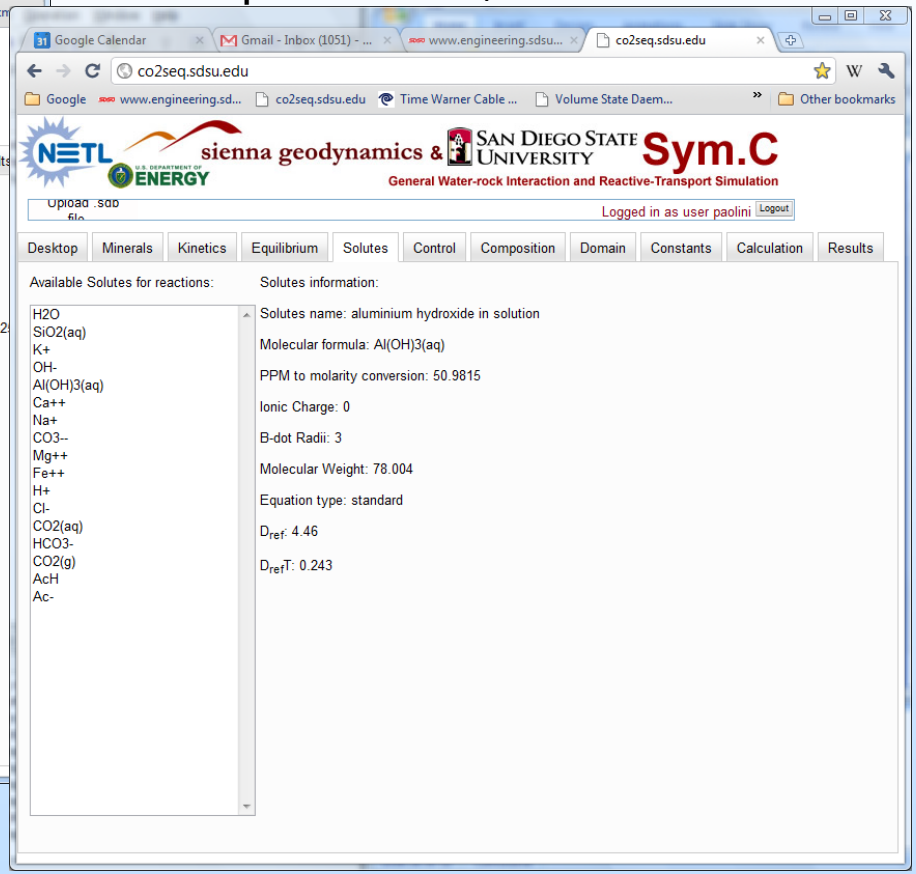


Equilibrium (relatively fast) reactions, solute specification, simulation control



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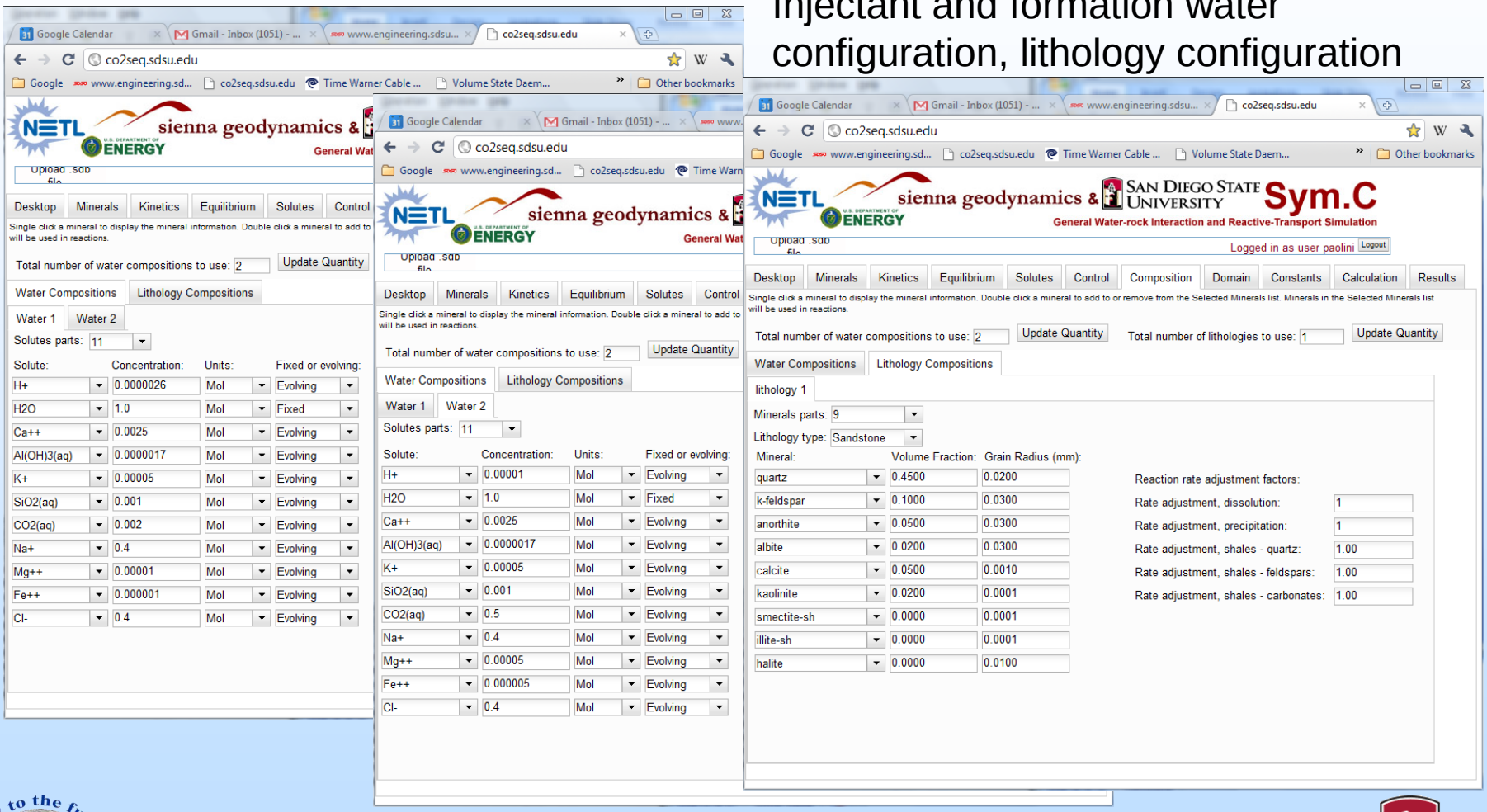
SOPO Goal #1: RIA for Simulating Water-Rock Interaction

Injectant and formation water configuration, lithology configuration



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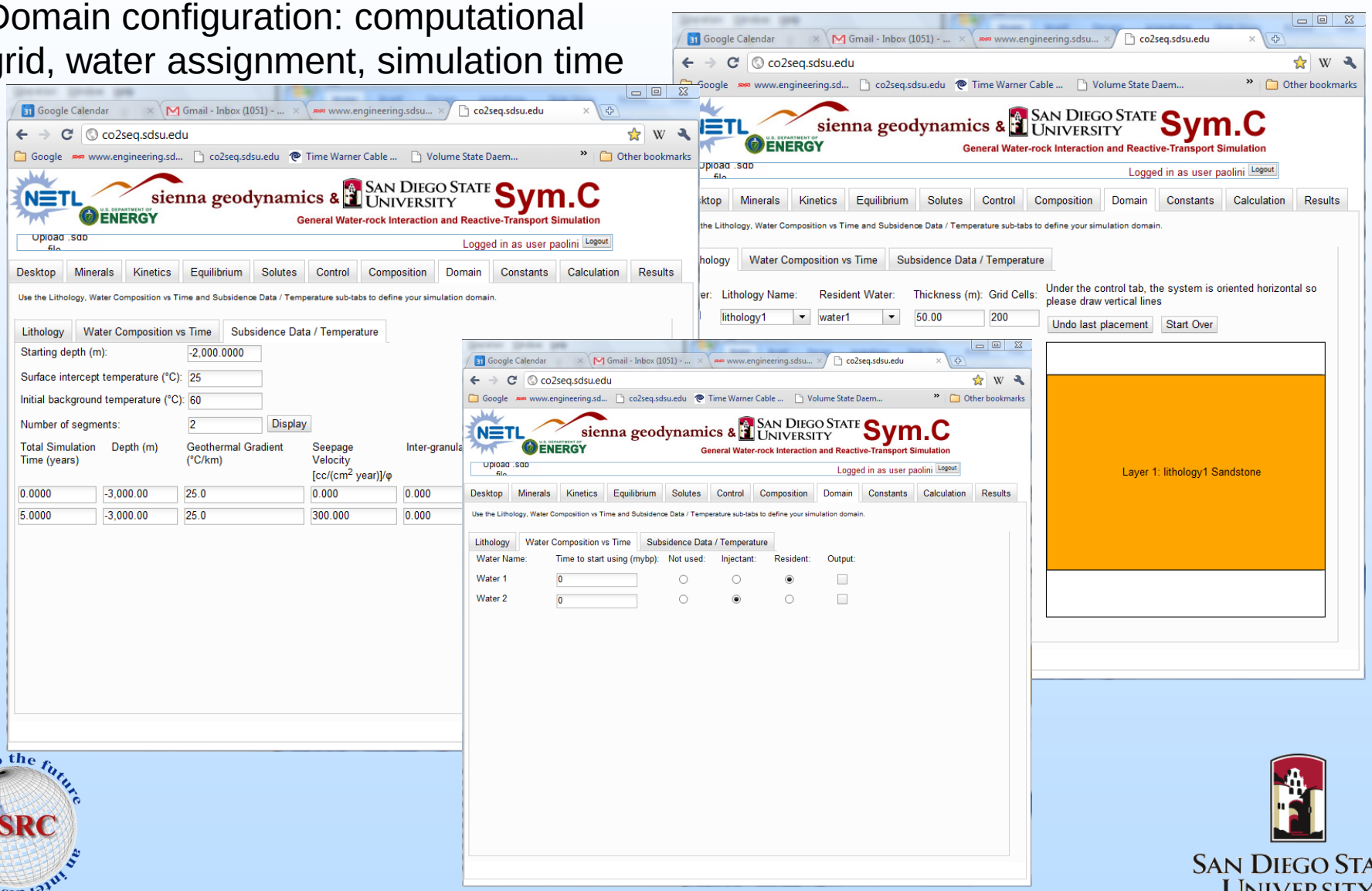
SOPO Goal #1: RIA for Simulating Water-Rock Interaction

Domain configuration: computational grid, water assignment, simulation time



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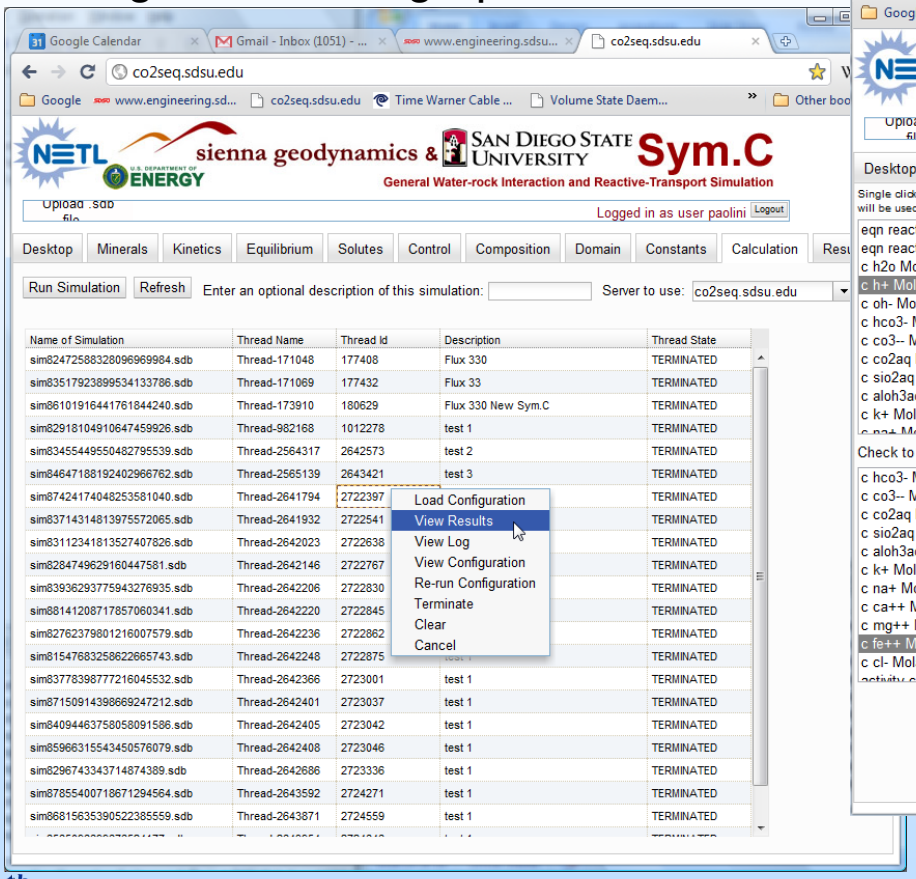
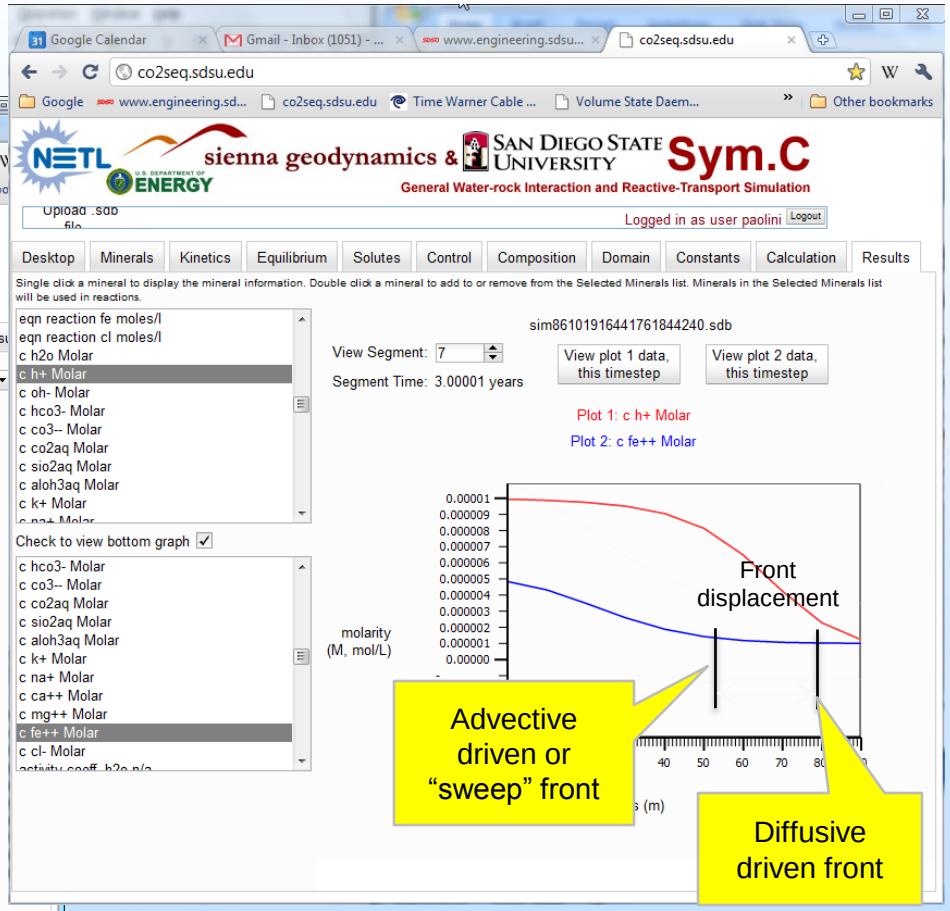
SOPO Goal #1: RIA for Simulating Water-Rock Interaction

Simulation invocation, status, management, and graphical results





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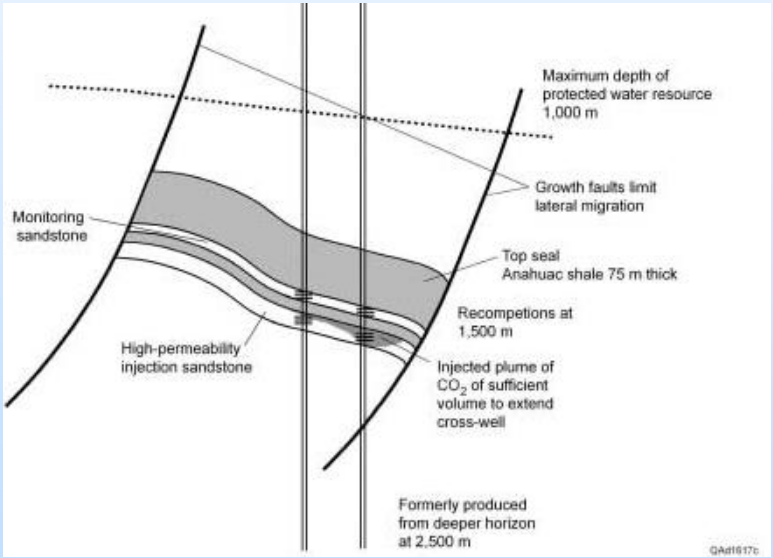
SOPO Goal #2: New Course on CO_2 Sequestration at SDSU

- I developed and successfully taught a new course entitled *Carbon Capture and Sequestration* at San Diego State University.
- Course took place during the fall semester of 2011 (August 22 through December 13) and meet twice a week on Tuesday and Thursday from 4:00 PM to 5:15 PM for 3 units of graded credit.
- The topics covered included brine water chemistry, cap rock chemistry, carbonaceous mineral reactions, geochemical redox reactions, thermodynamics fundamentals, the *Helgeson-Kirkham-Flowers* (HKF) model for computing thermodynamic properties of aqueous electrolytes, fundamentals of chemical kinetics, kinetics of mineral carbonation, and the computation of aqueous solute activities.
- RIA was used by the students to simulate various CCS scenarios and other geochemical processes (e.g. Liesegang banding in sandstone).

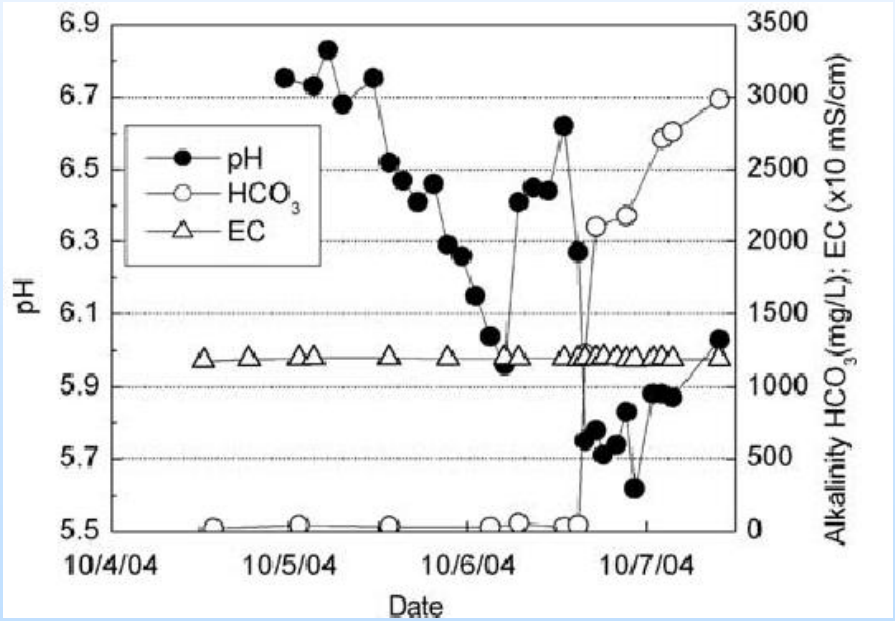
Technical Status

SOPO Goal #2: New Course on CO_2 Sequestration at SDSU

- Motivation for one problem: Frio Brine Pilot experiment showed a pH decrease before the arrival of HCO_3^-.
- Students asked to show if simulation showed same result and provide an explanation.



(Havorka and Knox, 2002)



(Y.K. Kharaka et al., 2006)

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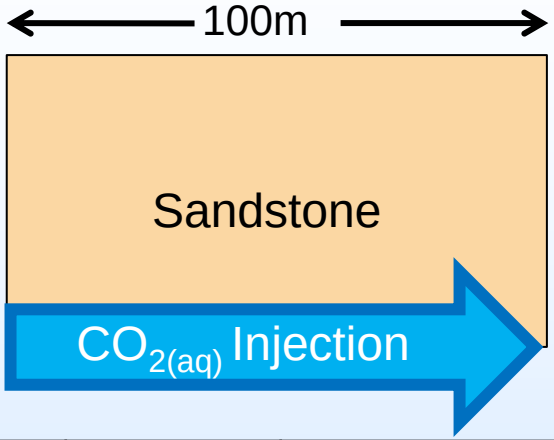
SOPO Goal #2: New Course on CO_2 Sequestration at SDSU

- 1D horizontal simulation (T = 20°C to 120°C).
- $CO_{2(aq)}$ injected at seepage velocities of 100, 200, 300, 400, and 500 [cc/(cm^2 yr)]/φ for 5 years.
- The CO_2-rich injectant water was modeled as a mixture of the formation water and 0.5M solutions of $CO_{2(aq)}$.
- Iron as tracer with 5x the molarity (non reactive).



Ion	Formation Water	Injectant Water
pH	5.59	5
CO2 (aq)	total 0.002M	Total 0.5M
HCO3-		
CO3--		
Ca++	0.0025 M	0.0025 M
Al(OH)3	1.7x10-6 M	1.7x10-6 M
K+	5.0x10-5 M	5.0x10-5 M
SiO2(aq)	0.001 M	0.001 M
Na+	0.4 M	0.4 M
Cl-	0.4 M	0.4 M
Fe++	1.0x10-5 M	5.0x10-5 M
Mg++	1.0X10-4 M	5.0x10-4 M

Mineral	Volume (%)	Grain Radii (cm)
Quartz	0.45	0.0200
k-feldspar	0.10	0.0300
Anorthite	0.05	0.0300
Albite	0.02	0.0300
Calcite	0.05	0.0010
Kaolinite	0.02	0.0001
Smectite	0.00	0.0001
Illite	0.00	0.0001
Halite	0.00	0.0100

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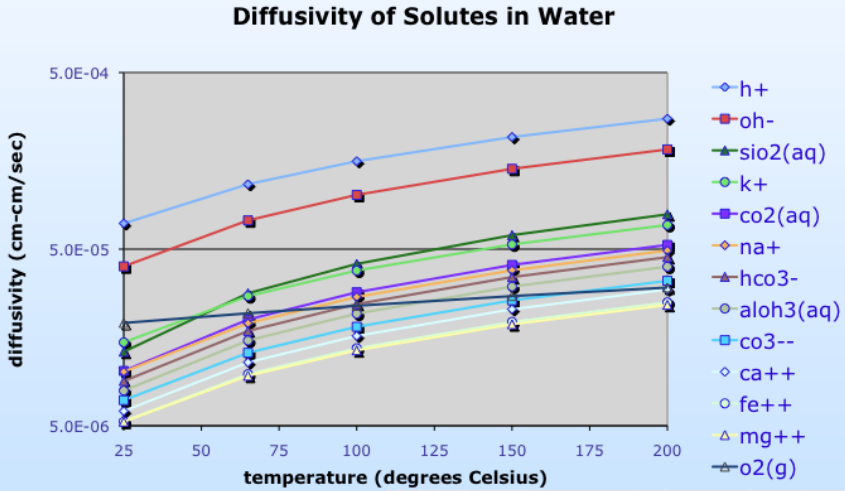
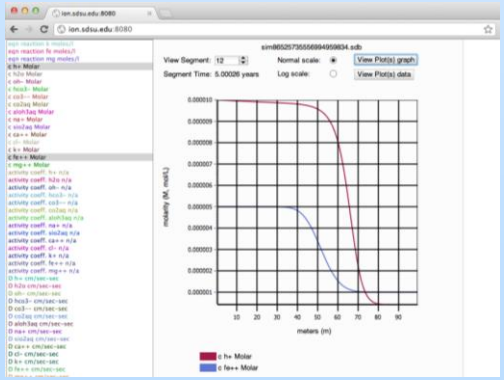
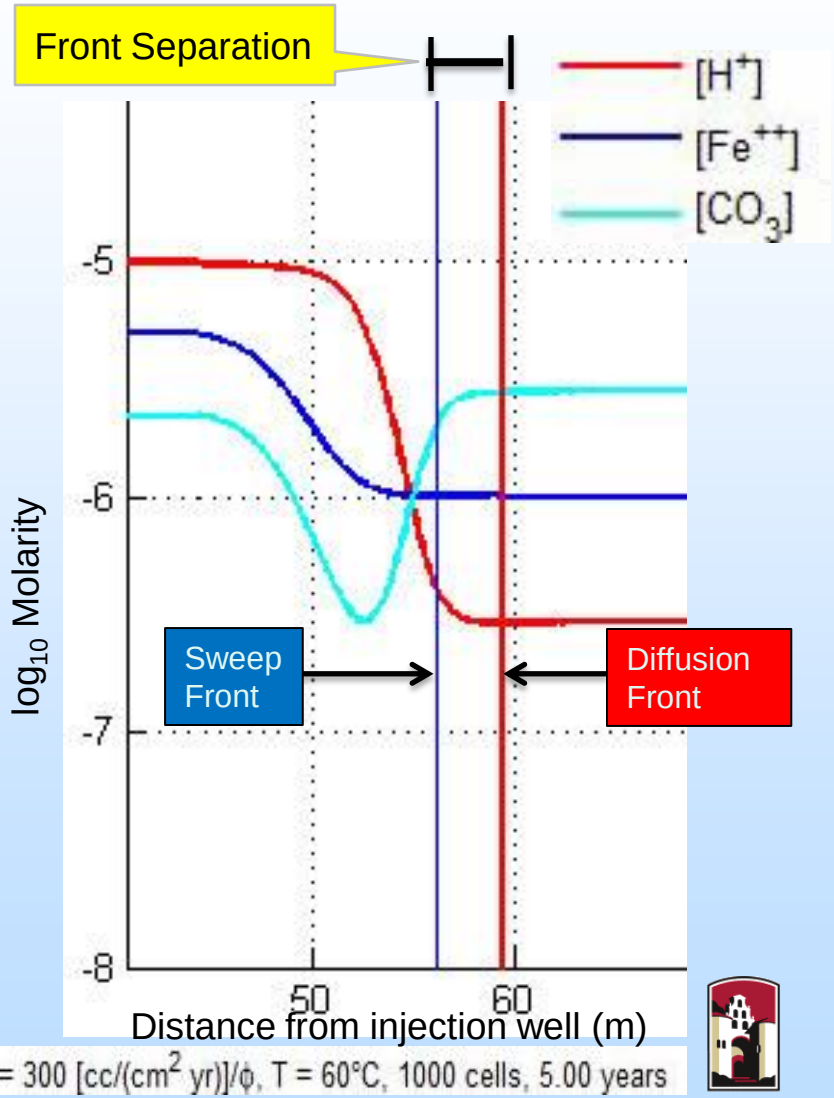
- Sweep (advective) front and diffusion front develop when CO_2-rich water displaces formation water.
- Differences in diffusivities of solutes are the most likely cause of the front separation.



Li and Gregory, 1974;
Boudreau, 1997





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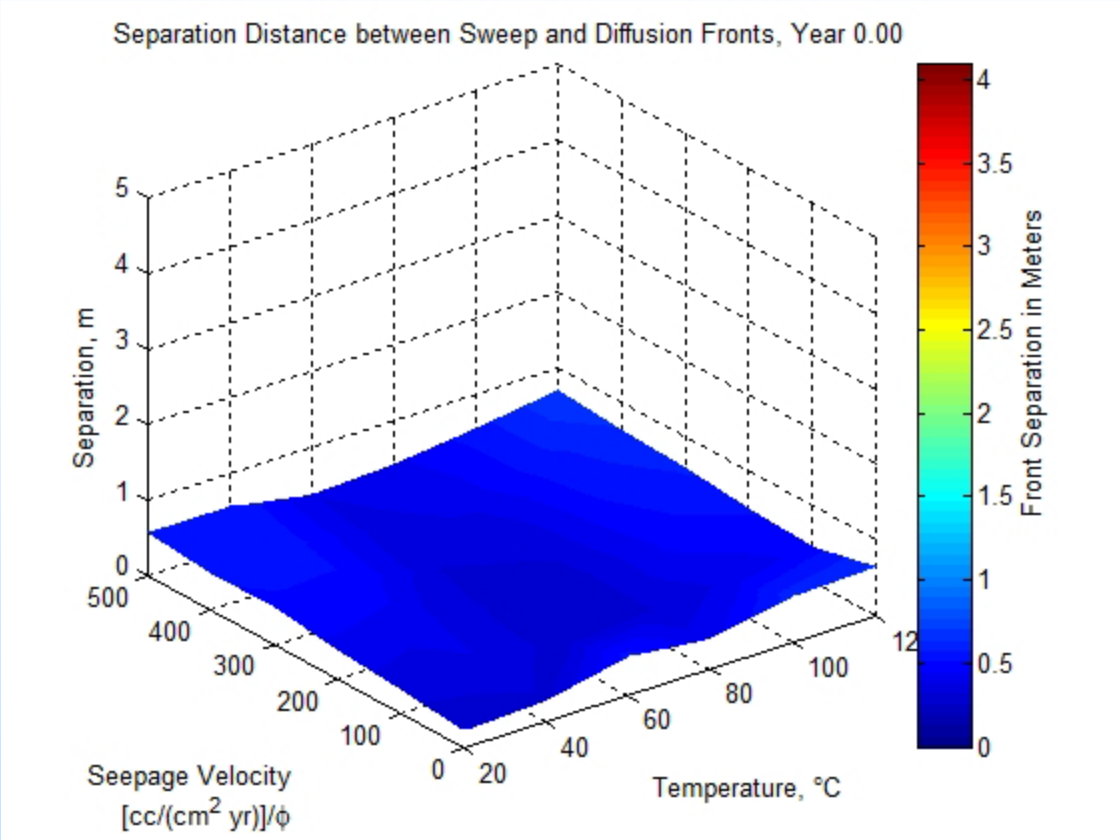
- Finding: separation distance changes in time as a function of reservoir temperature and seepage velocity.
- Front separation occurs when advective driven solute transport is less dominant than diffusive driven transport .
- Local minima at high temperatures and low injectant velocity.
- Maxima propagates to a lower temperature region over time.



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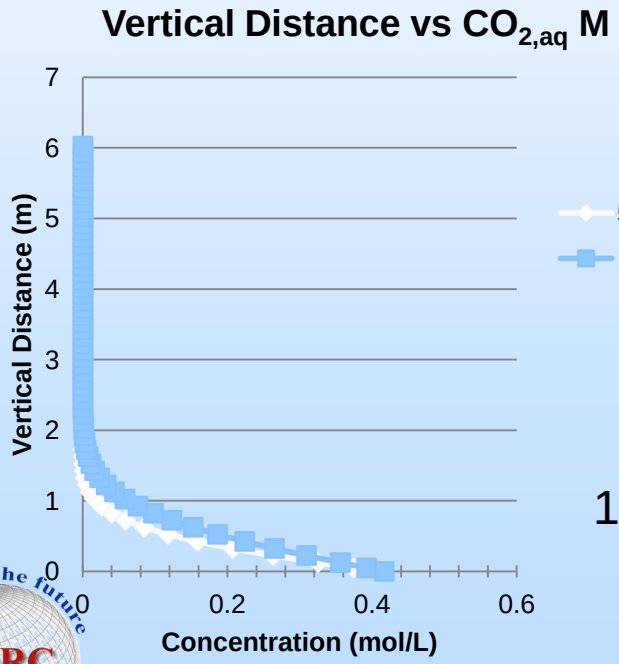
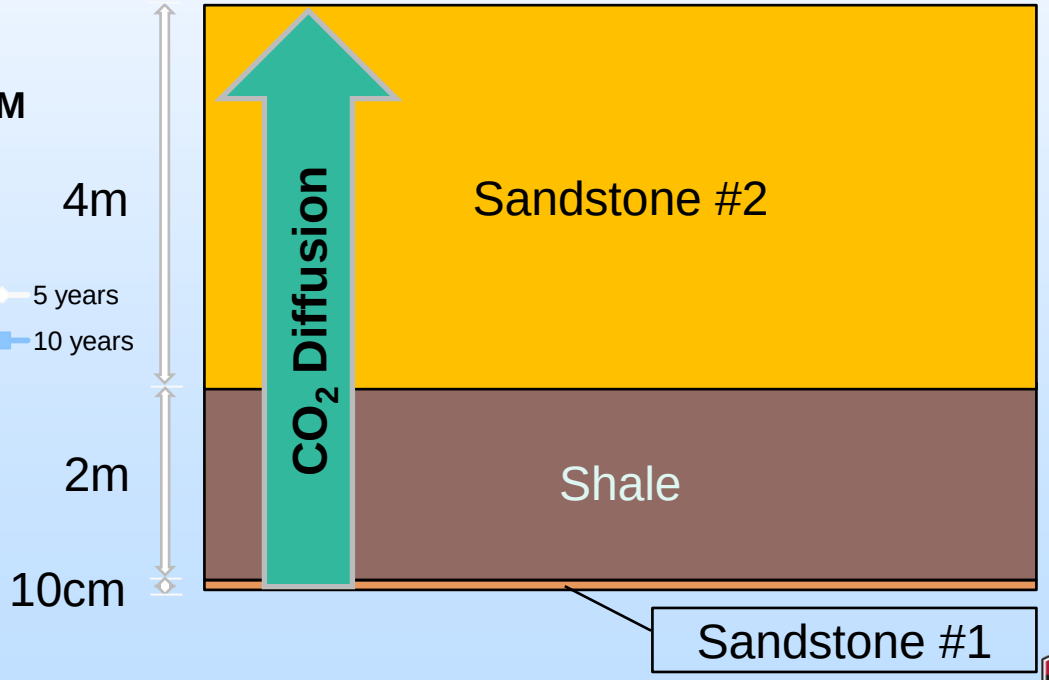
- Another problem: investigate vertical CO_2 diffusion through three different lithologies.
- Pure diffusion problem (seepage velocity v_x = 0 m/s)
- T_{res} = 60°C





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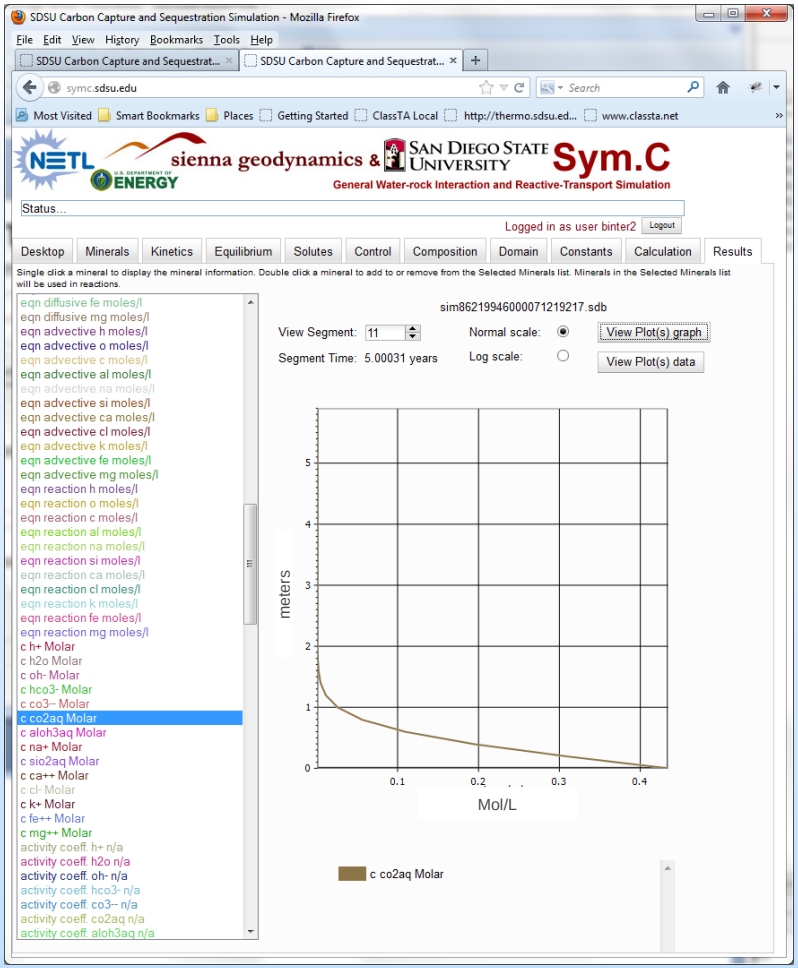

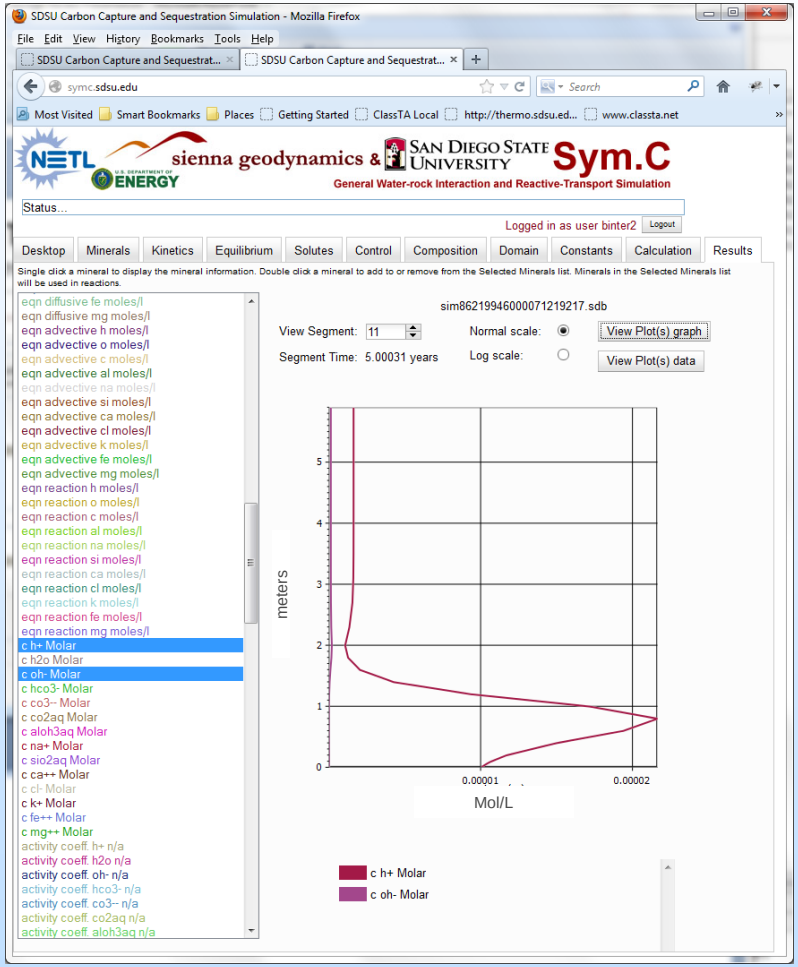

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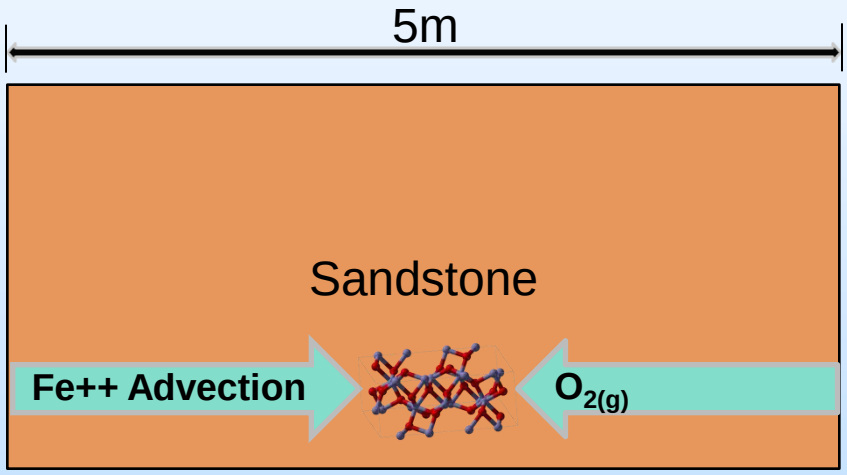
SOPO Goal #2: New Course on CO_2 Sequestration at SDSU

- Using the RIA to investigate Liesegang banding in sandstone.
- Asked students to investigate naturally occurring patterns of Hematite precipitation - iron(III) oxide (Fe_2O_3) over a 5m portion of sandstone.
- Configuration: seepage velocity v_x = 0.35 m/(yr φ), T_{res} = 60°C and D_{res} = 2000m
- Lithology:

Mineral	Volume Fraction	Grain Radius [mm]
quartz	0.65	0.02

- Water compositions

Solute	Formation, M	Backflow, M	Injectant, M
$SiO_{2(aq)}$	0.0001	0.0001	0.0001
H^+	2.1e-07	2.1e-07	1.1e-05
H_2O	1	1	1
$O_{2(g)}$	1.0e-08	1.0e-08	5.0e-14
Fe^{++}	4.0e-19	4.0e-19	6.6e-14



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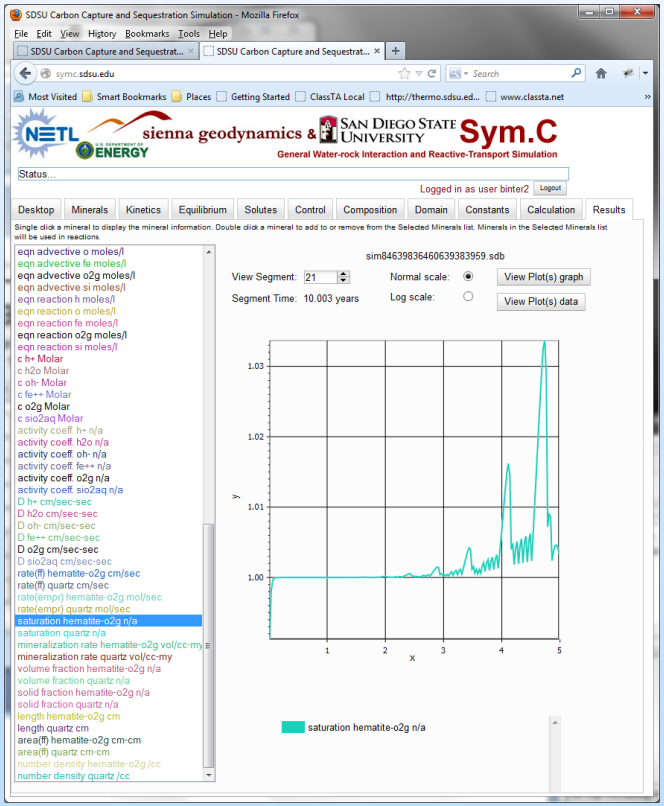
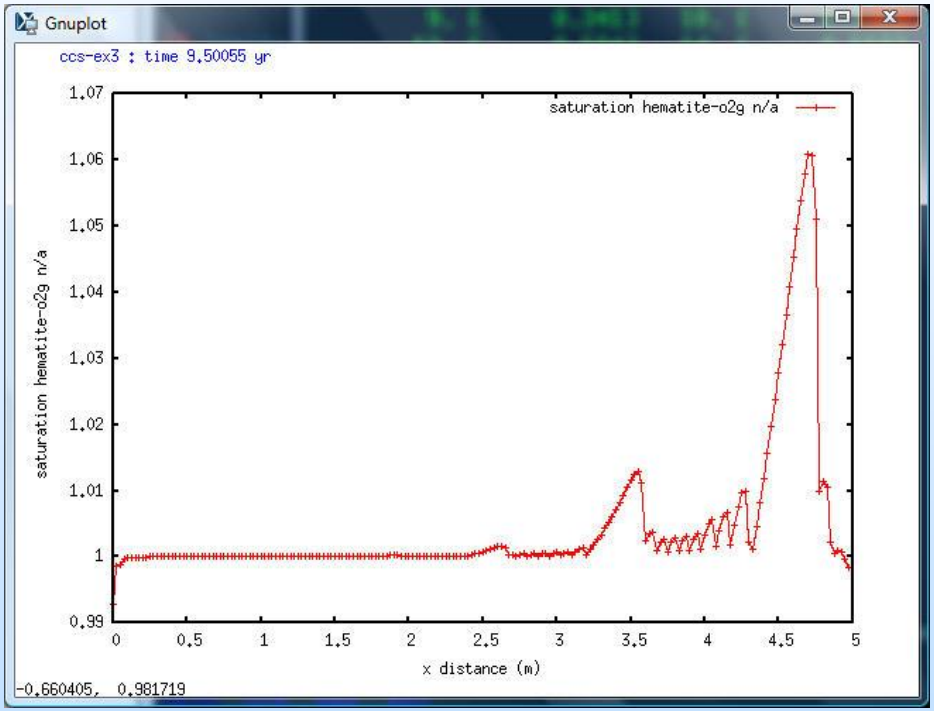
- By specifying a fairly large number (~200) of cells, the pattern formation becomes apparent after 10 years (Liesegang Banding).
- Precipitation occurs where hematite saturation >1





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SOPO Goal #3: Computational Science Program Development

- Three current graduate students: Christopher Binter, MS Geological Sciences; Eduardo J. Sanchez Peiro, PhD Computational Science; Jonathan L. Matthews, PhD Computational Science
- **Christopher Binter**: *heat transfer and multiphase fluid flow module*. Initial implementation solves a temperature advection-diffusion equation using Spalding and Patankar's Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm with source term calculated using the Helgeson-Kirkham-Flowers (HKF) model for computing thermodynamic properties of aqueous electrolytes.
- **Eduardo J. Sanchez Peiro**: *parallel mass transport solver*. Implementation of a parallel large-sparse system solver module to solve for solute concentrations in parallel on SDSC TeraGrid/XSEDE system *trestles.sdsu.edu* using SuperLU distributed solver developed at Lawrence Berkeley National Laboratory.
- **Jonathan L. Matthews**: *poroelastic pore pressure module*. Implementation of a discretized pore pressure diffusion model that computes the resultant mean stresses in rock. The calculated stresses used to investigate the occurrence and behavior of rock fractures during injection of $CO_{2,(aq)}$ into sandstone.

Technical Status

SOPO Goal #3: Computational Science Program Development

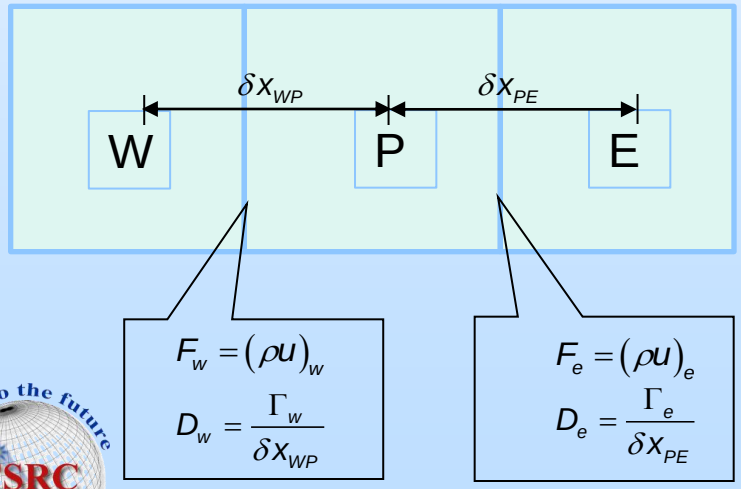
- Initial heat transfer module implementation: 1D transient advection-diffusion with source based on HKF model

$$\frac{\partial}{\partial t}(\rho T)+\frac{\partial}{\partial x}(\rho u T)=\frac{\partial}{\partial x}\left(\Gamma\frac{\partial T}{\partial x}\right)+S_T$$

$$(\rho u T)_e-(\rho u T)_w=\left(\Gamma\frac{\partial T}{\partial x}\right)_e-\left(\Gamma\frac{\partial T}{\partial x}\right)_w+S_T\Delta x$$

$$a_P T_P = a_W T_W + a_E T_E$$

$$a_p = a_W + a_E + \left(F_e - F_w\right) \qquad a_e = D_e - \frac{F_e}{2} \qquad a_w = D_w + \frac{F_w}{2}$$



$$D = \frac{G}{dx}\left[\frac{g}{m^2 s}\right]$$

$$G = \frac{k}{c_p}\left[\frac{g}{m\,s}\right]$$

k is thermal conductivity (W/(m·K))
c_p is specific heat capacity (J/(g·K))
dx is distance between grid centers

$$F = r\,u \quad \left[\frac{g}{m^2 s}\right]$$

r = Mixture Density $\left[\frac{g}{m^3}\right]$

u = seepage velocity $\left[\frac{m}{s}\right]$

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- The source term represents the energy generation as heat resulting from a change in solute concentration.

$$S_T = \sum_{j=1}^{n} \left(\frac{M_j}{c_{p,j(aq)}} \right)^{-1} \left(\frac{dc_j}{dt} \right) H_j; \quad \left[\frac{gK}{m^3 s} \right]$$

- Thermodynamic properties (molar heat capacity, molar volume, and molar enthalpy) of charged aqueous solute species computed using Helgeson-Kirkham-Flowers (HKF) Model.

$$\bar{c}_p = c_1 + \frac{c_2}{(T - \Theta)^2} - \frac{2T}{(T - \Theta)^3} \left[a_3 (P - P_r) + a_4 \ln \left(\frac{\Psi + P}{\Psi + P_r} \right) \right] + \omega T X + 2TY \left(\frac{\partial \omega}{\partial T} \right)_P - T(Z - 1) \left(\frac{\partial^2 \omega}{\partial T^2} \right)_P$$

- The relative permittivity (dielectric constant) of H_2O, the Born coefficient, and the Born functions are also calculated for a given temperature, pressure, and density.

Ψ = Solvent pressure (2600 bar)
Θ= Water singularity temperature (228K)
P_r = Reference pressure (1 bar)
P = Simulation pressure (bar)
T = Simulation temperature (K)

ω = Born coefficient (J/mol)
ε = Permittivity of H_2O (-)
Z, Y, X = Born functions (-), (1/K), ($1/K^2$)

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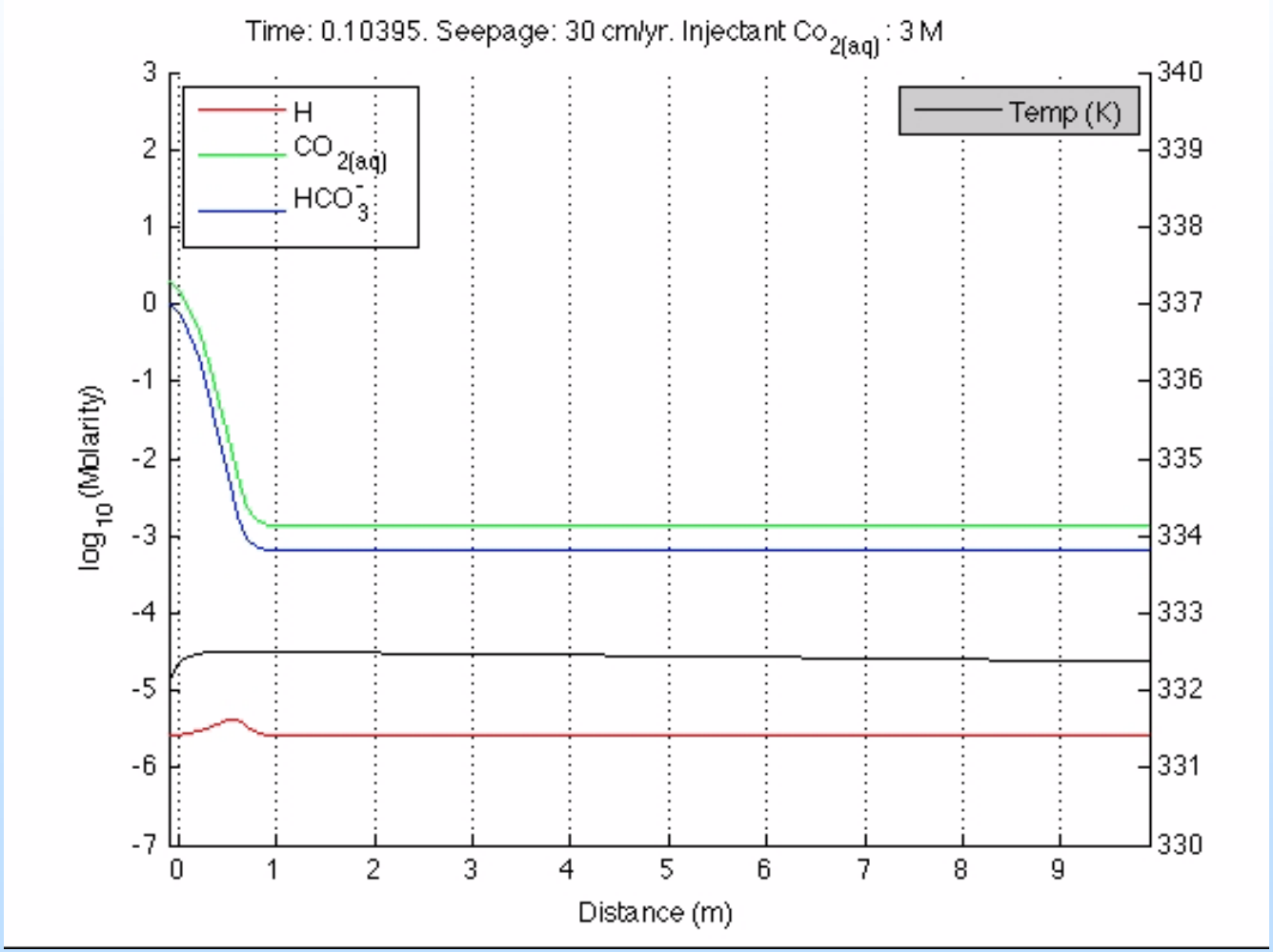
SOPO Goal #3: Computational Science Program Development

- Example result: v_x= 30cm/yr, $CO_{2(aq)}$ conc. = 3M, t = 1000yr, T_{res}= 59°C



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SOPO Goal #3: Computational Science Program Development

Elemental Conservation of Mass

$$\frac{\partial e_\beta}{\partial t} = \sum_{\alpha=1}^{Na} \nu_{\beta\alpha} \left[\phi D_\alpha \nabla^2 c_\alpha - \phi \vec{\nabla} \cdot \left(c_\alpha \vec{u} \right) \right] - \sum_{\gamma=1}^{M} \nu_{\beta\gamma} \rho_\gamma A_\gamma G_\gamma$$

Elemental mass rate of change term: rate of increase of concentration of a solute atom β in a fluid element

Diffusive term: net rate of increase of solute activity in a fluid element due to diffusive forces

Advective term: net rate of flow of solute activity out of a fluid element due to advective forces

Source term: net rate of the increase or decrease of a mineral in a fluid element due to chemical kinetics

• Evolution of chemical elemental mass depends on mass-transfer from diffusive and advective forces as well as the precipitation and dissolution of minerals governed by kinetic reaction rates

- f **porosity**
- D **diffusion coefficient**
- u **water flow velocity**
- n **reaction stoichiometry**
- A **mineral surface area**
- c **solute concentration**
- e **chemical elemental mass**
- G **mineral reaction rate**
- k **reaction rate constant**
- β **solute atom index**
- γ **mineral index**
- ρ_γ **mineral solid molar density**
- K **equilibrium constant**
- Ea **activation energy**
- R **gas constant**
- T **temperature**
- α **aqueous solute species index**

(A. J. Park)

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SOPO Goal #3: Computational Science Program Development

- Parallel mass transport solver implementation: parallel large-sparse system solver module to solve for solute concentrations in parallel on SDSC TeraGrid/XSEDE system *trestles.sdsu.edu* using SuperLU *distributed*, developed at Lawrence Berkeley National Laboratory.
- Mass-transfer coefficient matrices constructed from formation and injectant water velocities and solute concentrations, derived from the previous iteration, are structured and then solved using LU factorization.
- Formulation is not well suited for execution on many-core distributed clusters.
- New scheme: all solute concentrations in all control volumes are solved simultaneously by constructing a large block-banded sparse matrix.
- BLOGS: Block-defined Global Sparse Scheme

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- We define the following system of rank $N \times N_a$:

$$\begin{bmatrix} \mathbf{W}_{1,1} & \mathbf{W}_{1,2} & & & \cdots & & \mathbf{W}_{1,N} \\ \mathbf{B}^{w}_{2,1} & \mathbf{B}^{0}_{2,2} & \mathbf{B}^{e}_{2,3} & & & & \\ & \mathbf{B}^{w}_{3,2} & \mathbf{B}^{0}_{3,3} & \mathbf{B}^{e}_{3,4} & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \mathbf{B}^{w}_{i,j-1} & \mathbf{B}^{0}_{i,j} & \mathbf{B}^{e}_{i,j+1} & \\ & & & & \ddots & \ddots & \\ \mathbf{E}_{N,1} & & \cdots & & & \mathbf{E}_{N,N-1} & \mathbf{E}_{N,N} \end{bmatrix} \begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_2 \\ \mathbf{c}_3 \\ \vdots \\ \mathbf{c}_e \end{bmatrix} = \begin{bmatrix} \mathbf{r}(\mathbf{c}_w) \\ \mathbf{r}(\mathbf{c}_2) \\ \mathbf{r}(\mathbf{c}_3) \\ \vdots \\ \mathbf{r}(\mathbf{c}_e) \end{bmatrix}$$

$\mathbf{B}^{0}_{i,j}$ is a sparse, diagonal block of dimension $(N_a \times N_a)$ from discretization terms at the i-th node.

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$$
\begin{bmatrix}
\mathbf{W}_{1,1} & \mathbf{W}_{1,2} & & \cdots & & \mathbf{W}_{1,N} \\
\mathbf{B}^{w}_{2,1} & \mathbf{B}^{0}_{2,2} & \mathbf{B}^{e}_{2,3} & & & \\
 & \mathbf{B}^{w}_{3,2} & \mathbf{B}^{0}_{3,3} & \mathbf{B}^{e}_{3,4} & & \\
 & & \ddots & \ddots & \ddots & \\
 & & & \mathbf{B}^{w}_{i,j-1} & \mathbf{B}^{0}_{i,j} & \mathbf{B}^{e}_{i,j+1} & \ddots \\
 & & & & \ddots & \ddots & \\
\mathbf{E}_{N,1} & & \cdots & & \mathbf{E}_{N,N-1} & \mathbf{E}_{N,N}
\end{bmatrix}
\begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_2 \\ \mathbf{c}_3 \\ \vdots \\ \mathbf{c}_e \end{bmatrix}
=
\begin{bmatrix} \mathbf{r}(\mathbf{c}_w) \\ \mathbf{r}(\mathbf{c}_2) \\ \mathbf{r}(\mathbf{c}_3) \\ \vdots \\ \mathbf{r}(\mathbf{c}_e) \end{bmatrix}
$$

$\mathbf{B}^{w}_{i,j-1}$ and $\mathbf{B}^{e}_{i,j+1}$ are both sparse and diagonal blocks of dimension $(N_a \times N_a)$ from discretization terms at both the west-neighboring (w) node and the east-neighboring (e) node.

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$$\begin{bmatrix} \mathbf{W}_{1,1} & \mathbf{W}_{1,2} & & & \cdots & & \mathbf{W}_{1,N} \\ \mathbf{B}^{w}_{2,1} & \mathbf{B}^{0}_{2,2} & \mathbf{B}^{e}_{2,3} & & & & \\ & \mathbf{B}^{w}_{3,2} & \mathbf{B}^{0}_{3,3} & \mathbf{B}^{e}_{3,4} & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \mathbf{B}^{w}_{i,j-1} & \mathbf{B}^{0}_{i,j} & \mathbf{B}^{e}_{i,j+1} & \\ & & & & \ddots & \ddots & \ddots \\ \mathbf{E}_{N,1} & & \cdots & & & \mathbf{E}_{N,N-1} & \mathbf{E}_{N,N} \end{bmatrix} \begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_2 \\ \mathbf{c}_3 \\ \vdots \\ \mathbf{c}_e \end{bmatrix} = \begin{bmatrix} \mathbf{r}(\mathbf{c}_w) \\ \mathbf{r}(\mathbf{c}_2) \\ \mathbf{r}(\mathbf{c}_3) \\ \vdots \\ \mathbf{r}(\mathbf{c}_e) \end{bmatrix}$$

$\mathbf{W}_{1,1}$ to $\mathbf{W}_{1,N}$ are sparse and diagonal blocks of dimension $(N_a \times N_a)$ from discretization terms at both the west boundary. These comprise the first N_a rows of the matrix.

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$$
\begin{bmatrix}
\mathbf{W}_{1,1} & \mathbf{W}_{1,2} & & & \cdots & & \mathbf{W}_{1,N} \\
\mathbf{B}^{w}_{2,1} & \mathbf{B}^{0}_{2,2} & \mathbf{B}^{e}_{2,3} & & & & \\
 & \mathbf{B}^{w}_{3,2} & \mathbf{B}^{0}_{3,3} & \mathbf{B}^{e}_{3,4} & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & \mathbf{B}^{w}_{i,j-1} & \mathbf{B}^{0}_{i,j} & \mathbf{B}^{e}_{i,j+1} & \\
 & & & & \ddots & \ddots & \ddots \\
\mathbf{E}_{N,1} & & \cdots & & & \mathbf{E}_{N,N-1} & \mathbf{E}_{N,N}
\end{bmatrix}
\begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_2 \\ \mathbf{c}_3 \\ \vdots \\ \mathbf{c}_e \end{bmatrix}
=
\begin{bmatrix} \mathbf{r}(\mathbf{c}_w) \\ \mathbf{r}(\mathbf{c}_2) \\ \mathbf{r}(\mathbf{c}_3) \\ \vdots \\ \mathbf{r}(\mathbf{c}_e) \end{bmatrix}
$$

$\mathbf{E}_{N,N}$ to $\mathbf{E}_{N,1}$ are sparse and diagonal blocks of dimension $(N_a \times N_a)$ from discretization terms at both the east boundary. These comprise the last N_a rows of the matrix.

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$$
\begin{bmatrix}
\mathbf{W}_{1,1} & \mathbf{W}_{1,2} & & & \cdots & & \mathbf{W}_{1,N} \\
\mathbf{B}^{w}_{2,1} & \mathbf{B}^{0}_{2,2} & \mathbf{B}^{e}_{2,3} & & & & \\
 & \mathbf{B}^{w}_{3,2} & \mathbf{B}^{0}_{3,3} & \mathbf{B}^{e}_{3,4} & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & \mathbf{B}^{w}_{i,j-1} & \mathbf{B}^{0}_{i,j} & \mathbf{B}^{e}_{i,j+1} & \\
 & & & & \ddots & \ddots & \ddots \\
\mathbf{E}_{N,1} & & \cdots & & & \mathbf{E}_{N,N-1} & \mathbf{E}_{N,N}
\end{bmatrix}
\begin{bmatrix}
\mathbf{c}_w \\ \mathbf{c}_2 \\ \mathbf{c}_3 \\ \vdots \\ \mathbf{c}_e
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{r}(\mathbf{c}_w) \\ \mathbf{r}(\mathbf{c}_2) \\ \mathbf{r}(\mathbf{c}_3) \\ \vdots \\ \mathbf{r}(\mathbf{c}_e)
\end{bmatrix}
$$

$\mathbf{c}_i$ is the vector of length N_a of all the concentration variables at node i.

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$$
\begin{bmatrix}
\mathbf{W}_{1,1} & \mathbf{W}_{1,2} & & & \cdots & & \mathbf{W}_{1,N} \\
\mathbf{B}^{w}_{2,1} & \mathbf{B}^{0}_{2,2} & \mathbf{B}^{e}_{2,3} & & & & \\
 & \mathbf{B}^{w}_{3,2} & \mathbf{B}^{0}_{3,3} & \mathbf{B}^{e}_{3,4} & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & \mathbf{B}^{w}_{i,j-1} & \mathbf{B}^{0}_{i,j} & \mathbf{B}^{e}_{i,j+1} & \\
 & & & & \ddots & \ddots & \ddots \\
\mathbf{E}_{N,1} & & \cdots & & & \mathbf{E}_{N,N-1} & \mathbf{E}_{N,N}
\end{bmatrix}
\begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_2 \\ \mathbf{c}_3 \\ \vdots \\ \mathbf{c}_e \end{bmatrix}
=
\begin{bmatrix} \mathbf{r}(\mathbf{c}_w) \\ \mathbf{r}(\mathbf{c}_2) \\ \mathbf{r}(\mathbf{c}_3) \\ \vdots \\ \mathbf{r}(\mathbf{c}_e) \end{bmatrix}
$$

$\mathbf{r}(\mathbf{c}_i)$ is a vector of length N_a of all the contributions from considered reactions, also at node i.

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SOPO Goal #3: Computational Science Program Development

- Poroelastic pore pressure module. Implementation of a discretized pore pressure diffusion model that computes the resultant mean stresses in rock. The calculated stresses used to investigate the occurrence and behavior of rock fractures during injection of $CO_{2,(aq)}$ into sandstone.

- Pressure diffusion follows the following non-homogeneous diffusion equation.

$$\frac{\partial p}{\partial t} - c\nabla^2 p = -\frac{\alpha}{S}\frac{dg}{dt} + \frac{Q}{S}$$

α – **Biot-Willis Coefficient**, relates fluid gain relative to increases in strain under constant pore pressure

S – **Uniaxial specific storage**, relates fluid gain to increases in pore pressure under uniaxial strain conditions

Q – **Fluid source**, rate fluid is added to a given reference volume per unit time not due to poroelastic flow

- However, in the case of an irrotational displacement field with the boundary conditions that ε, σ_{kk}, and p vanish at an infinite boundary, the integrating constant g(t) is identically zero, so the equation simplifies to:

$$\frac{\partial p}{\partial t} - c\nabla^2 p = \frac{Q}{S}$$

c – **Uniaxial hydraulic diffusivity**, controls the rate of pore pressure diffusion $(\frac{k}{\mu S})$

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- Using a first order implicit time derivative and a second order derivative in x, we discretize the equation as follows

$$\frac{p_j^{n+1} - p_j^n}{\Delta t} - c\frac{p_{j-1}^{n+1} - 2p_j^{n+1} + p_{j+1}^{n+1}}{(\Delta x)^2} = \frac{Q(x_j, t_{n+1})}{S}$$

- From this discretization, we get the following equations for the interior nodes:

$$p_j^n = rp_{j-1}^{n+1} + (1-2r)p_j^{n+1} + rp_j^{n+1} - \Delta t f(x_j, t_{n+1})$$

where $r = c\frac{\Delta t}{\Delta x^2}$ and $f(x_j, t_{n+1}) = \frac{Q(x_j, t_{n+1})}{S}$.

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SOPO Goal #4: Provide Industry with Trained Graduates

- Through this research grant, Christopher Binter has gained important and useful knowledge on CO_2 sequestration, carbonate mineralization, and reactive transport modeling.
- Knowledge gained directly from this grant determined his selection to be a summer intern at ExxonMobil where he is presently researching carbonate reefs in the North Caspian Sea.

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SOPO Goal #4: Provide Industry with Trained Graduates

- Eduardo J. Sanchez Peiro was accepted into the highly competitive Research Experience in Carbon Sequestration (RECS) 2012 program that was held June 3-13 in Birmingham, Alabama.
- RECS is a DOE/NETL sponsored intensive 10-day summer program that fosters and advances education, scientific research, professional training, and career networks for graduate students and young professionals in the carbon capture, utilization and storage (CCUS) field (http://www.recsco2.org/).
- Through the direct training and research experience Eduardo has gained from participating in this project**,** Eduardo was chosen to attend this year's RECS program.

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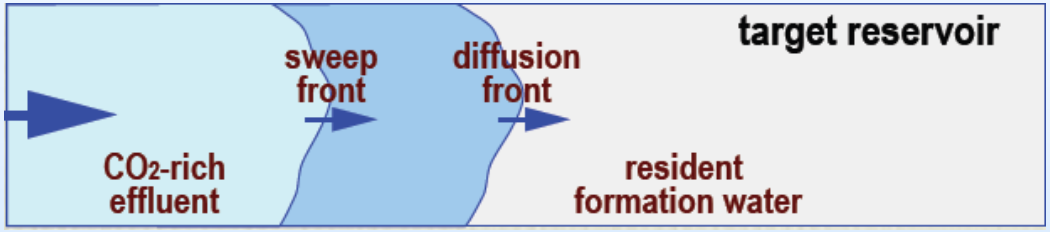
Accomplishments to Date

- Created a university-industry partnership with Sienna Geodynamics that has allowed SDSU to develop an intuitive Web interface to a water-rock interaction code that reduces the learning curve for geology and chemistry students to model and simulate typical CCS scenarios.
- Interface allows users to rapidly prototype 1D aqueous CO_2 injection into formation consisting of multiple lithologies, and then quickly pose *what-if* questions.
- Database includes support for many minerals, kinetic and “equilibrium” reactions, arbitrary number of fluid mixtures with many supported aqueous solute species.
- Licensing arrangement with Sienna Geodynamics has allowed SDSU to extend provided code to develop heat transfer and poroelastic pore-pressure modules and implement a novel new parallel solute mass transport scheme suitable for execution on TeraGrid/XSEDE systems.
- Development of new course at SDSU that focuses on the computational geochemistry of CO_2 sequestration.
- Successful placement of students into internships and research programs.

Summary

- Key Findings: Initial experimentation with Web interface in the classroom, used to model the Frio Pilot Test, has shown the injection front is preceded by an acidic front that develops as a result of different solute diffusivities.
- The acidic front, marked by an increase in H^+ concentration, could have an adverse effect on lithologies and seals.

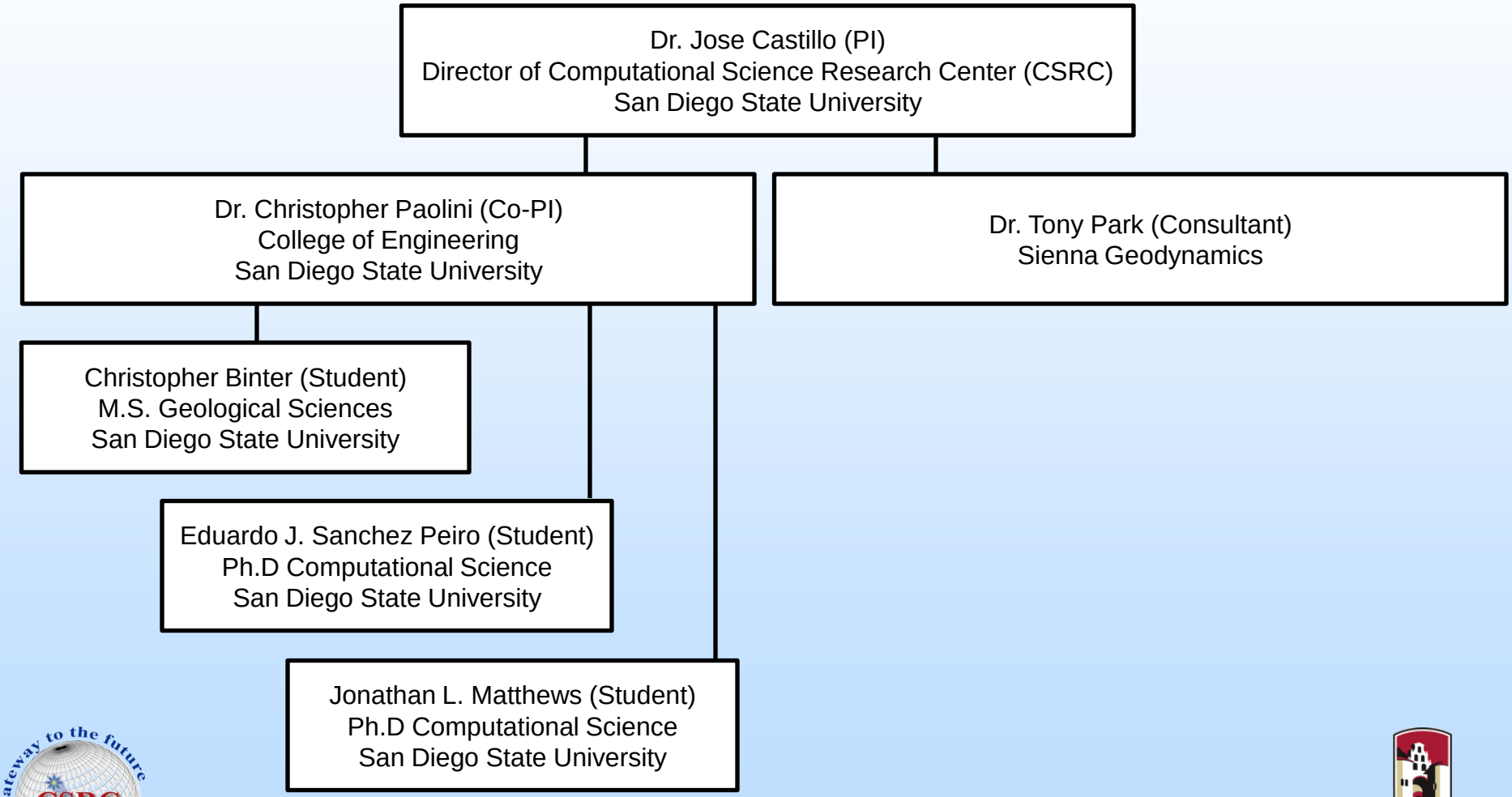


- Since solute diffusion and mineralization rates are temperature dependent, we are currently working on adding a heat transfer module to our simulator to capture changes in formation water temperature that occur during CO_2 injection.
- Lessons Learned: positive results using the Helgeson-Kirkham-Flowers (HFK) model to compute thermodynamic properties of aqueous electrolytes needed for the source term in the heat transfer model.
- Future Plans: Implementation of 2D and 3D mass and heat transport, support for multiphase flow (supercritical CO_2, oil, and gas phases), comparison with results from TOUGHREACT and STOMP.

Appendix

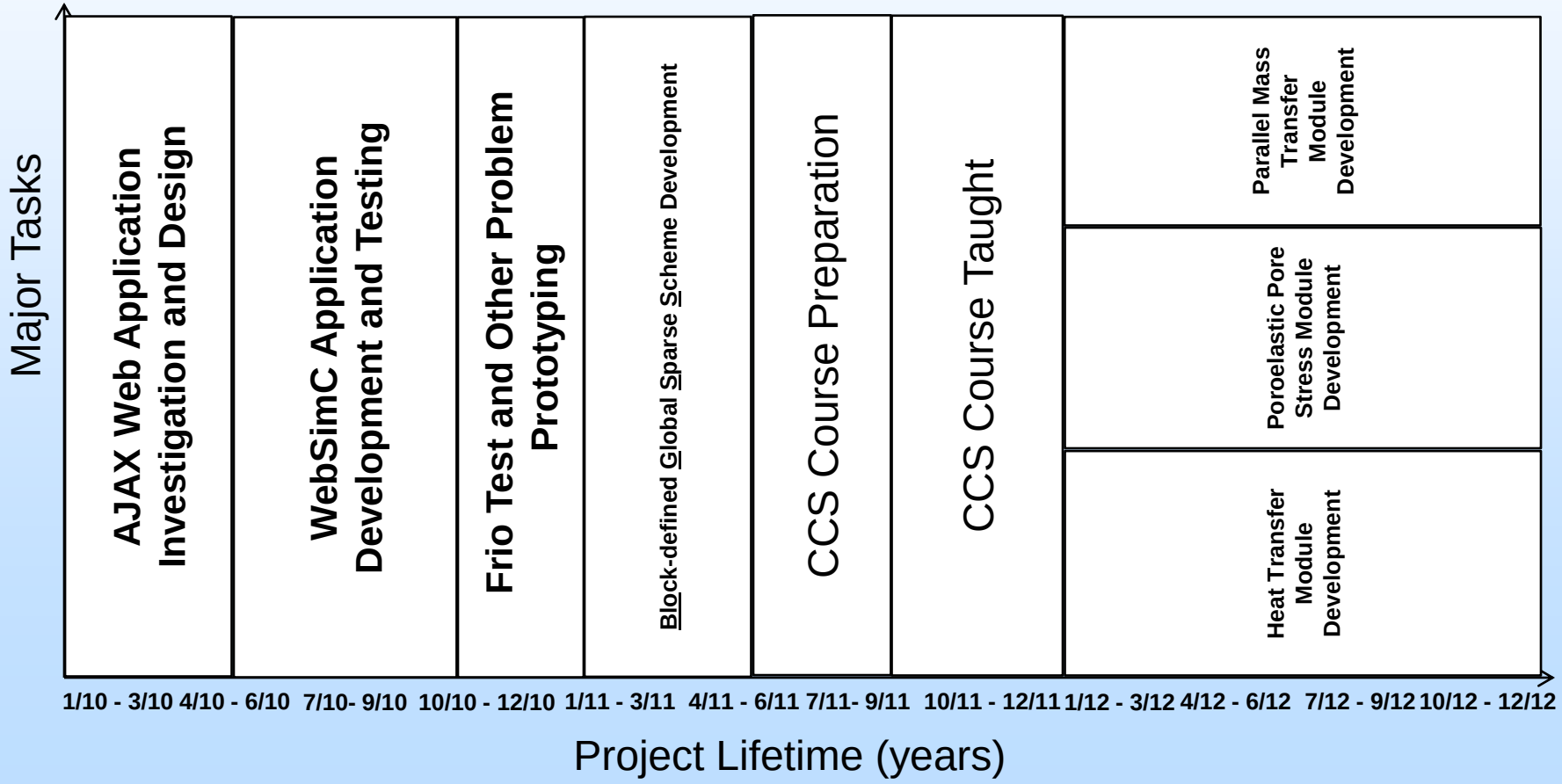
– These slides will not be discussed during the presentation, but are mandatory

Organization Chart



Gantt Chart

- Simple Gantt chart showing project lifetime in years on the horizontal axis and major tasks along the vertical axis.



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