


WESTCARB Annual Business Meeting

WESTCARB Phase III: Initial Modeling



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Outline

- **Approach**
 - The TOUGH codes
 - Hysteresis
- **Kimberlina Pilot**
 - Model geometry
 - Discretization
 - Results of preliminary modeling
- **Discussion Questions**



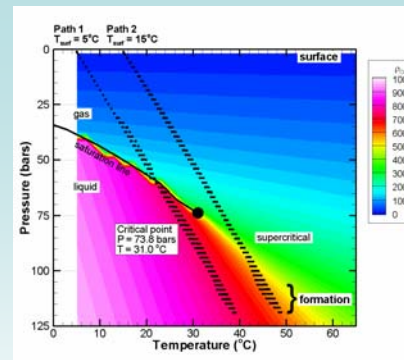
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The TOUGH Codes

- Multi-phase, multi-component fluid flow, tracer transport, and heat flow through porous or fractured media
- Integral finite difference method for space discretization
- Implicit time-stepping with Newton-Raphson iteration
- Several Equation of State (EOS) packages relevant for geologic CO₂ storage
- Additional modules for coupled processes
 - TOUGHREACT adds chemical reactions (contact: Tianfu Xu)
 - TOUGH-flac adds rock mechanics (contact: Jonny Rutqvist)
- Additional capabilities
 - TOUGH+ re-engineering of TOUGH codes (contact: George Moridis)
 - iTOUGH2 inverse model (contact: Stefan Finsterle)
 - TOUGH2/ECO2 with hysteretic capillary pressure and relative permeability formulations (contact: Christine Doughty)
 - TOUGH2/EOS7C for natural gas reservoirs (contact: Curt Oldenburg)
 - System-level simulations using TOUGH2 in the GoldSim framework (contact: Yingqi Zhang)

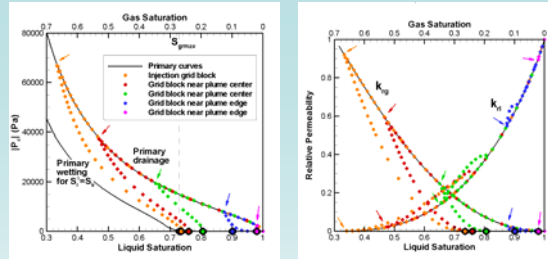
ECO2N

- EOS for CO₂ sequestration
- Components:
 - CO₂
 - H₂O
 - NaCl
- Phases
 - Supercritical
 - CO₂ rich, but may contain water vapor
 - ECO2N can gradually transition into gas
 - cannot cross the saturation line
 - Aqueous
 - H₂O rich, but may contain dissolved NaCl and CO₂
 - density dependence on dissolved species included
 - Solid
 - Includes precipitated NaCl
 - Solid formation decreases porosity and permeability



Pruess, K., Soc. Pet. Eng. J., 9(2), 237-248, 2004 (SPE-86098).

Hysteresis

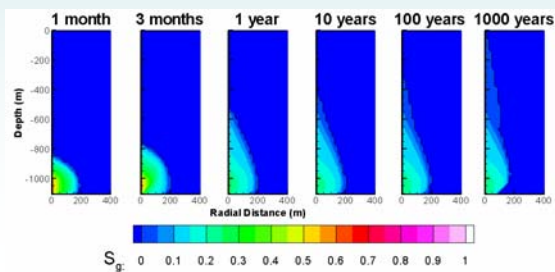
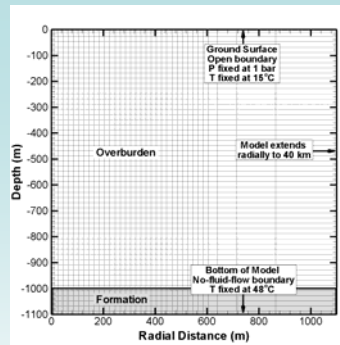


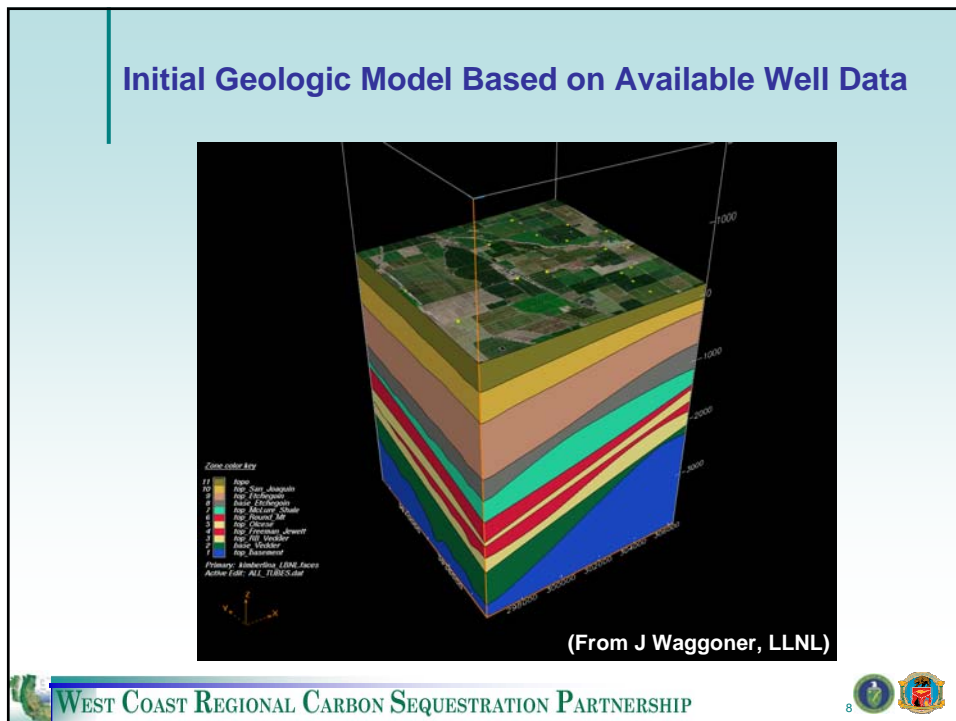
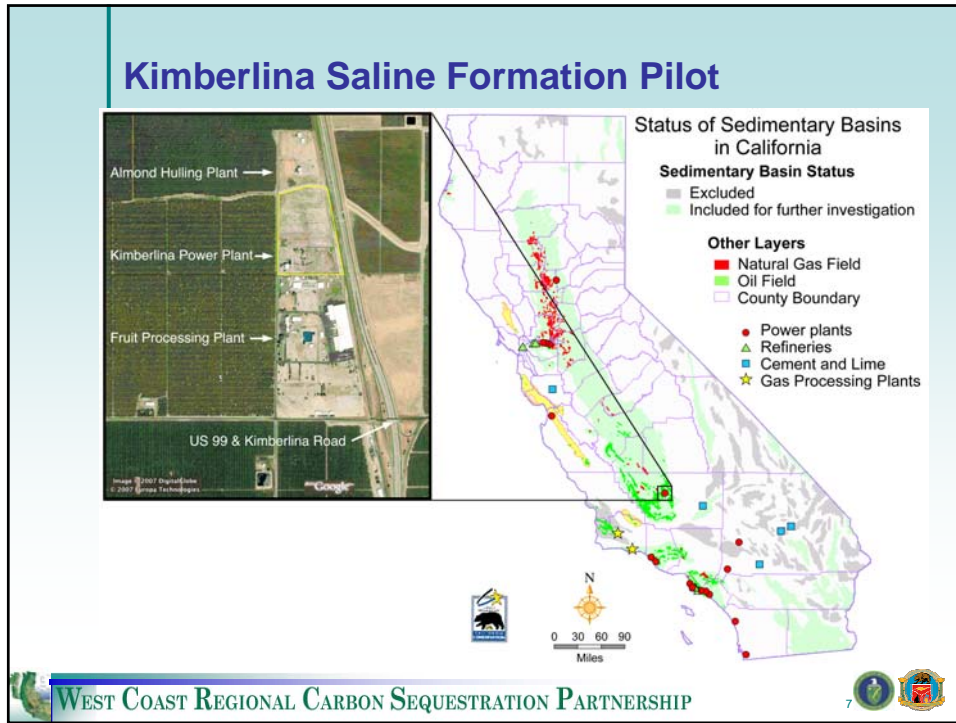
- Capillary pressure and relative permeability are history dependent
- Key feature is S_{gr} residual gas saturation (saturation below which CO_2 is immobile)
 - Drainage (CO_2 replaces brine): S_{gr} is zero
 - Imbibition (brine replaces CO_2): S_{gr} is non-zero and increases with maximum historic saturation
- Important for problems including both CO_2 injection and rest periods
 - Injection: all drainage
 - Rest: drainage at leading edge of plume, imbibition at trailing edge

Doughty, C., Modeling geologic storage of carbon dioxide: Comparison of non-hysteretic and hysteretic characteristic curves, Energy Conversion and Management, 48(6), 1768-1781, 2007.

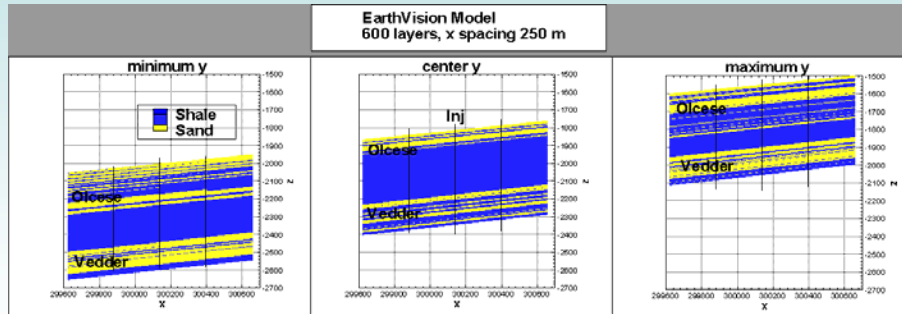
Hysteresis (cont'd)

- One month CO_2 injection at 1000-1100 m depth
- Watch plume for 1000 years
- High-permeability overburden (100 md)
- Leading edge of plume continues to move upward, but most of plume remains trapped at depth





Cross-Sections Through Sand-Shale Model

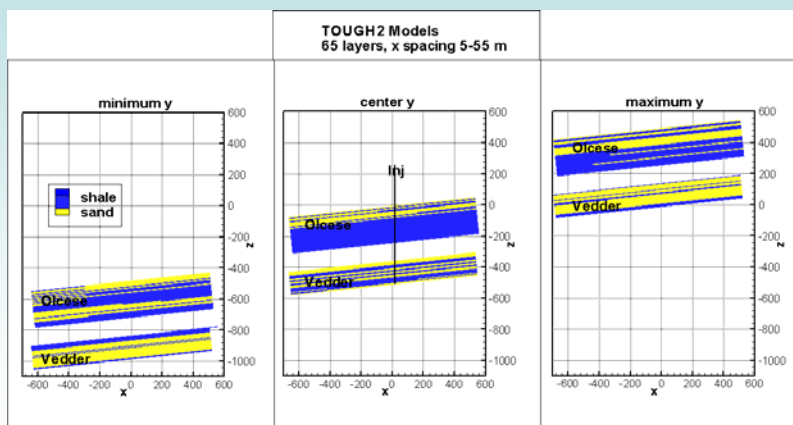


From J Waggoner, LLNL

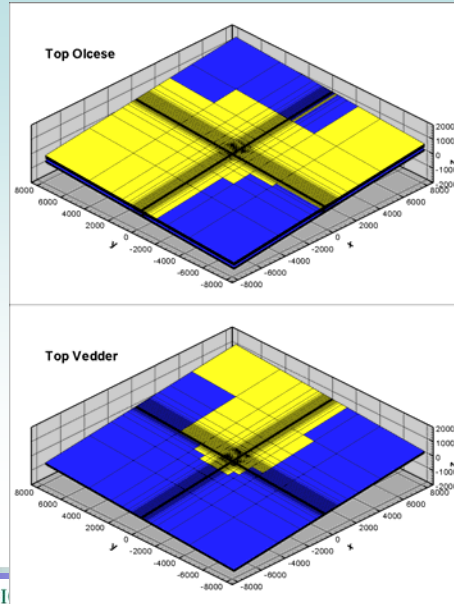
- Geologic model will be revised based on 3D seismic, core well logs



TOUGH2 Model Cross-Sections



TOUGH2 Models



TOUGH2 Model Development

- EarthVision model of Olcese and Vedder
 - 600 layers
 - 50 x 50 lateral cells
 - x: 250 m wide, y: 200 m wide
- TOUGH2 model
 - Olcese - 35 layers (8 EV layers combined to form each TOUGH2 layer)
 - Vedder - 30 layers (6 EV layers combined to form each TOUGH2 layer)
 - Closed boundaries above and below Olcese and Vedder
 - Constant-pressure boundaries at x extrema, closed at y extrema
 - Lateral grid spacing varies
 - 5 m at injection well
 - 55 m over region where CO₂ plume expected to go
 - Increasing to 2.5 km far from injection well
 - Earthvision facies assigned to TOUGH2 cells
 - Model is a tilted plane – good approximation to the nearly uniform dip observed in the EarthVision model. Dip angle is 7 degrees.

Model Parameters

Facies	Porosity	Horizontal Permeability	Vertical Permeability	Residual Liquid Saturation	Maximum Residual Gas Saturation
Sand	28%	200 md	20 md	0.2	0.277
Shale	15%	0.1 md	0.01 md	0.4	0.28

- Residual gas saturation
 - zero during drainage
 - non-zero during imbibition, depends on saturation history



Simulated Cases

- CO₂ Injection over full thickness of Vedder (158 m)
- CO₂ Injection over full thickness of Olcese (245 m)
- CO₂ Injection in uppermost Vedder sand body (25 m)

- Notes on Vedder and Olcese communication
 - Continuous shale
 - Thickness >100 m
 - Assume no communication
 - Can use separate models for each formation

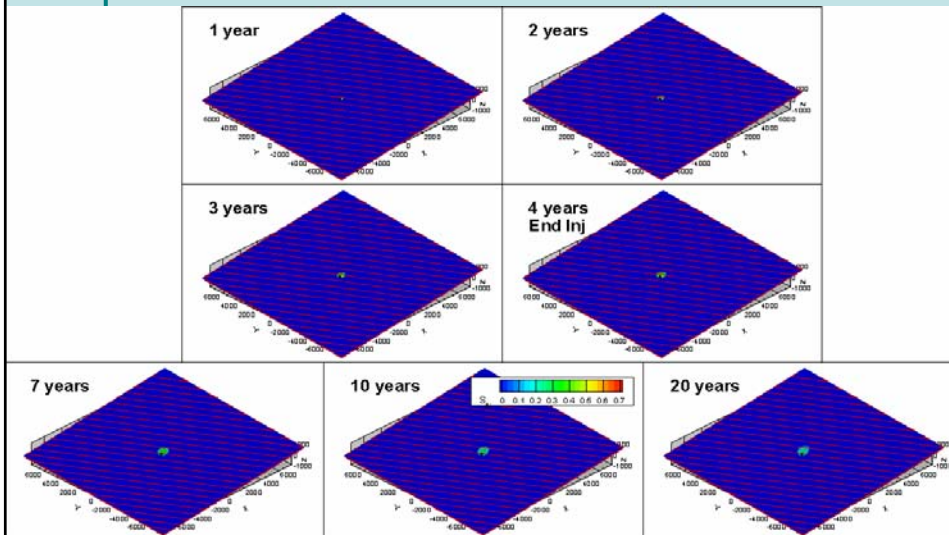


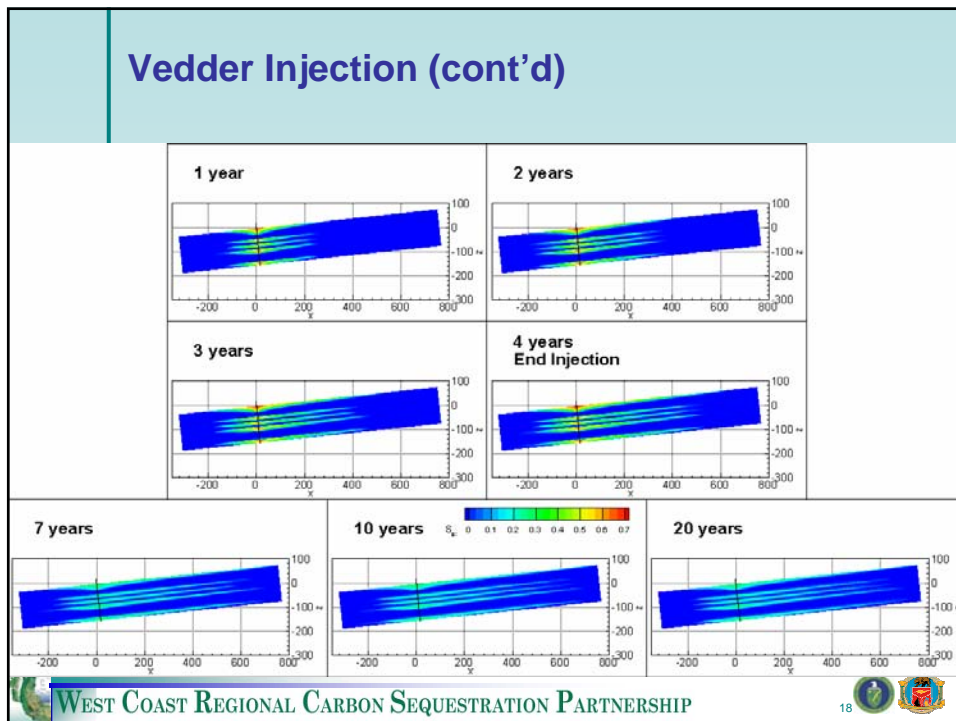
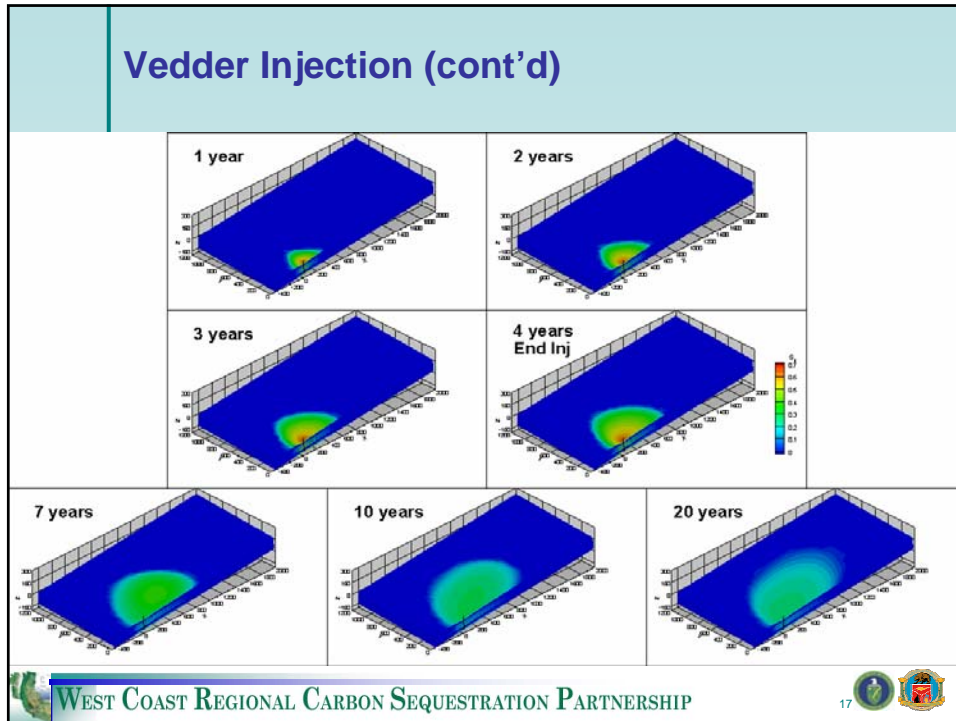
CO₂ Injection in Vedder

- Inject 250,000 t per year for 4 years
- Pick a central location in model for injection well
- Inject over entire thickness of Vedder (158 m thick)
- At injection location, about 50/50 sand/shale, so net sand thickness is about 79 m
- P = 220 bar, T = 81°C, density of CO₂ = 632 kg/m³



Vedder Injection



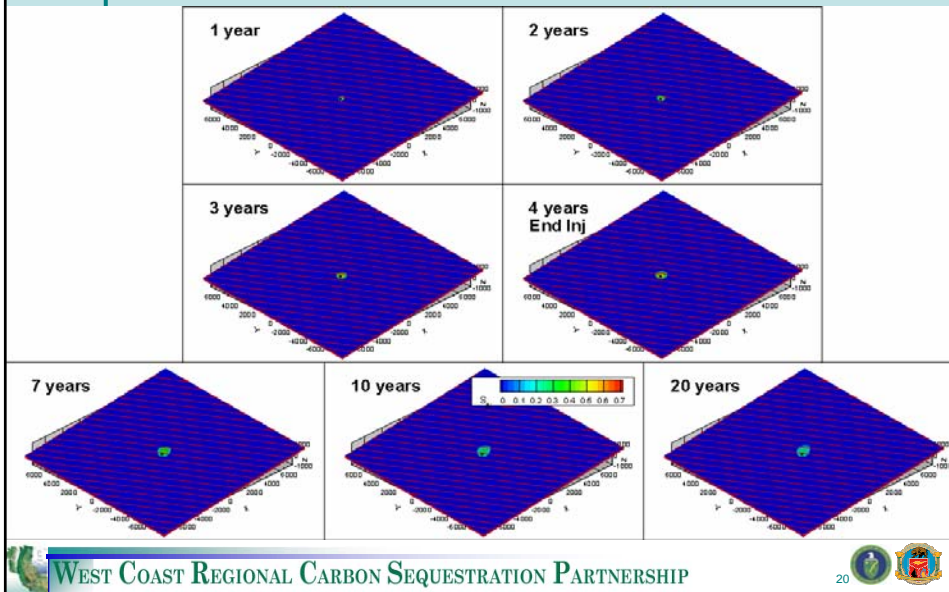


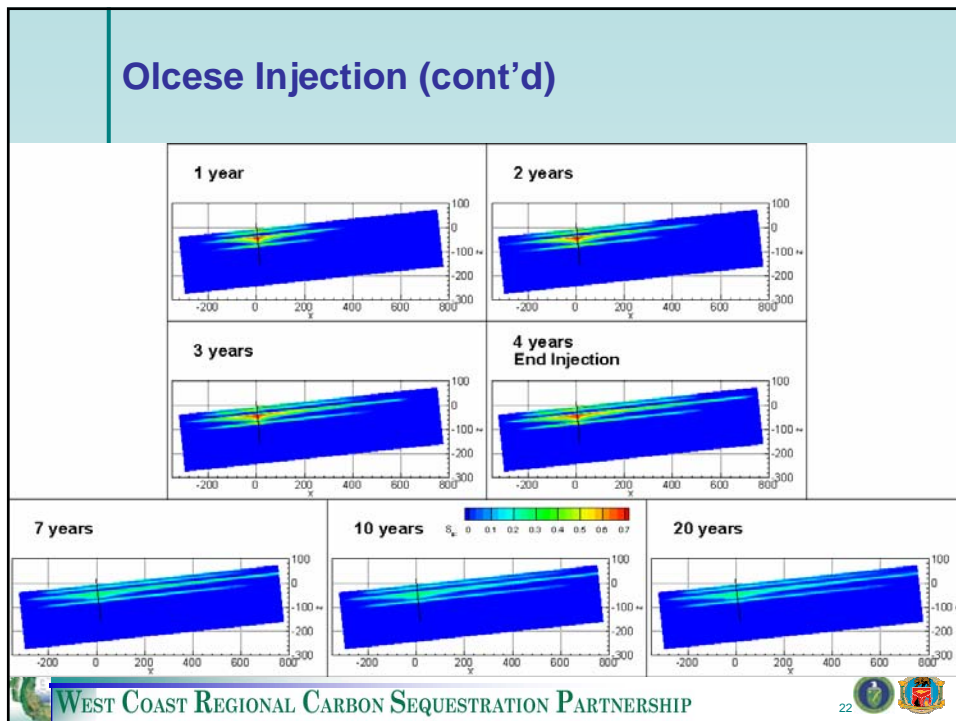
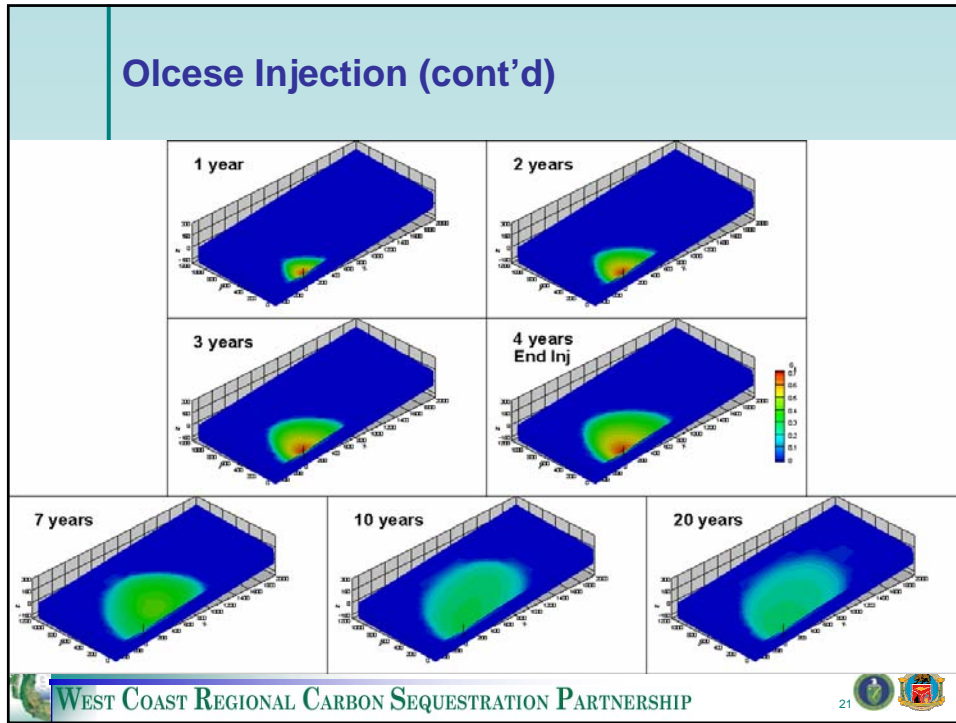
CO₂ Injection in Olcese

- Inject 250 kt per year for 4 years
- Pick a central location in model for injection well
- Nominally, inject over entire thickness of Olcese (245 m thick)
- At injection location, sand is all in upper third of formation, net sand thickness is about 50 m
- P = 180 bar, T = 69°C, density of CO₂ = 621 kg/m³



Olcese Injection



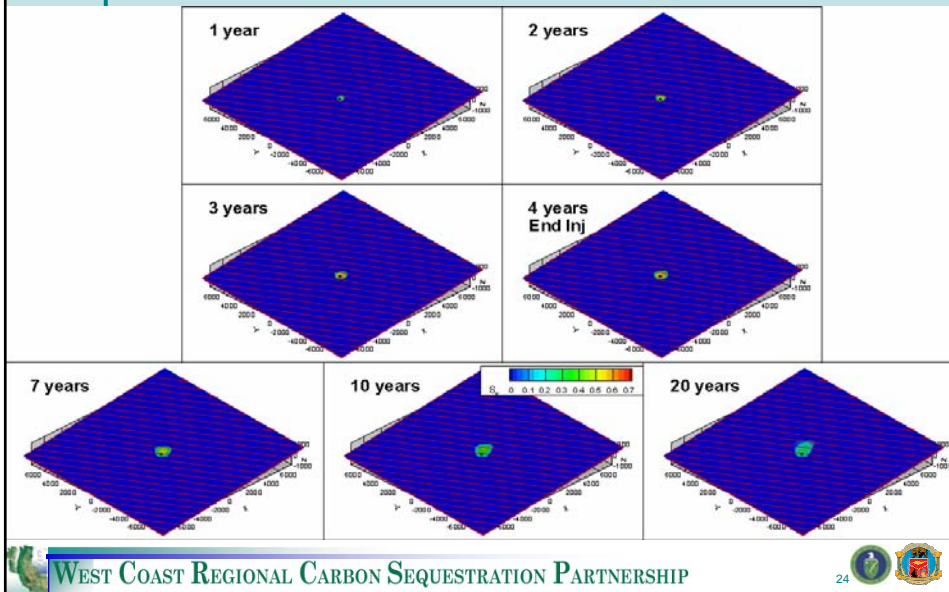


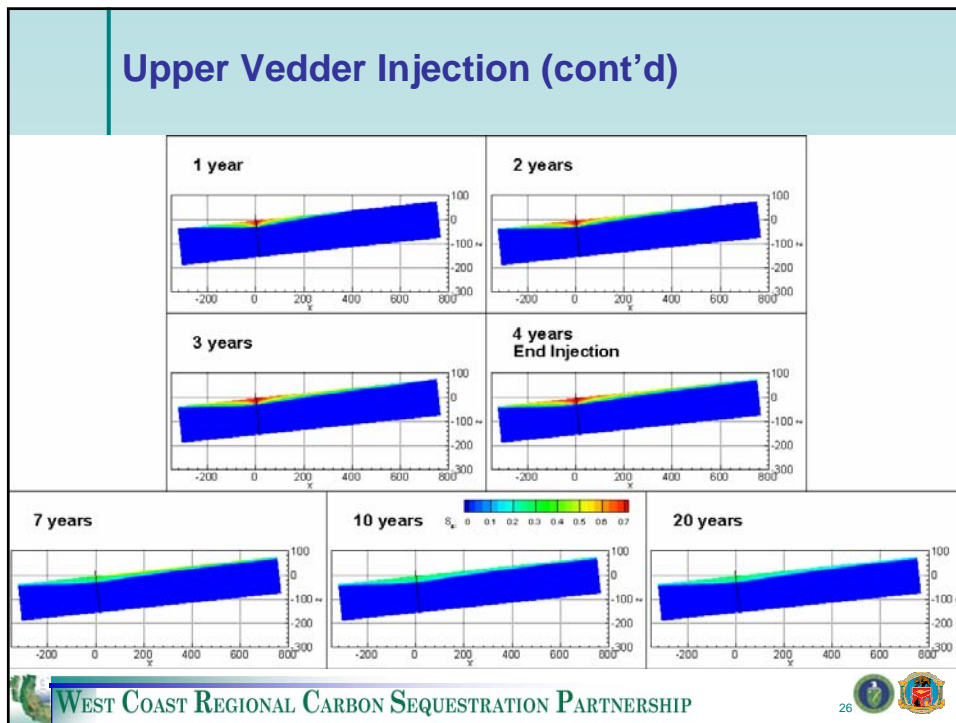
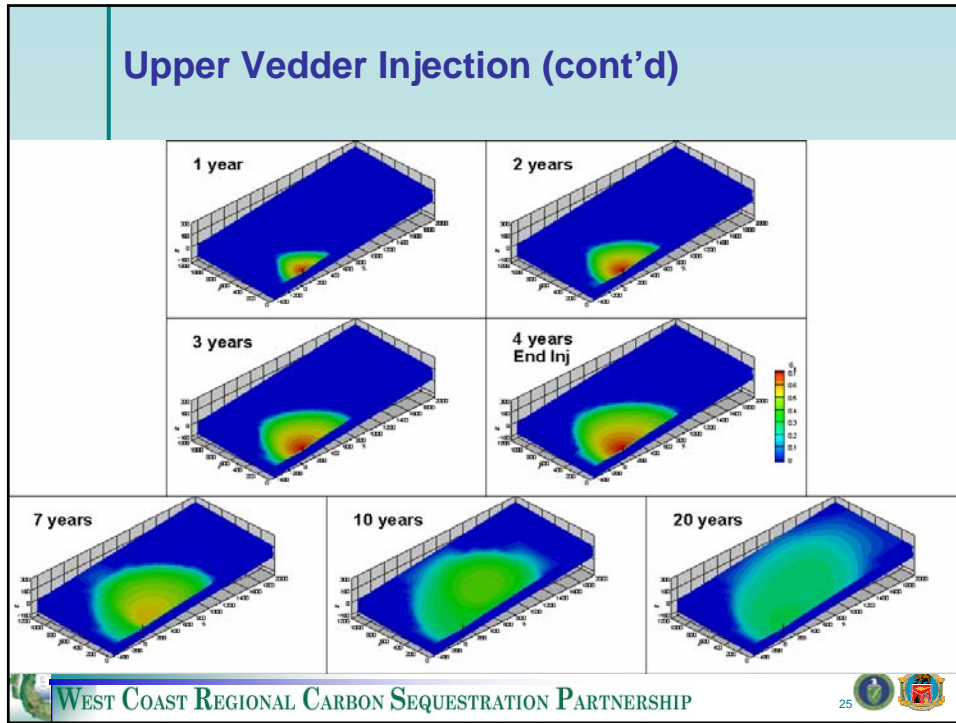
CO₂ Injection in Upper Vedder

- Inject 250 kt per year for 4 years
- Pick a central location in model for injection well
- Inject over uppermost sand body within Vedder (25 m thick)
- P = 220 bar, T = 81°C, density of CO₂ = 632 kg/m³



Upper Vedder Injection





Summary

- **Modeling is needed to predict plume migration and design CO₂ storage systems**
- **The TOUGH codes are available for a wide variety of CO₂-related modeling needs**
- **Application of TOUGH2/ECO2N with a preliminary version of the Kimberlina geologic model suggests plume size is small relative to the geologic model, but large relative to the property lines of the site**



Discussion

- **How do we use these results for Phase III?**
- **How will predictive results be used in general?**
 - **Needs of project proponent**
 - **Needs of regulators and public**
- **What can we do in Phase III to inform future projects?**
- **As more detailed information becomes available, how do we incorporate or update models and the uses to which results have been put?**



Acknowledgments

This work was supported in part by WESTCARB through the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, National Energy Technology Laboratory (NETL), and by Lawrence Berkeley National Laboratory under Department of Energy Contract No. DE-AC02-05CH11231.



WebGasEOS

LBNL interactive online application

The screenshot shows the WebGasEOS web application interface. On the left, there are input fields for EOS (Peng-Robinson), Temperature (200 °C), Pressure (100 bar), and a list of species (Methane, Ethane, Propane, Carbon Dioxide, Hydrogen Sulfide, Nitrogen, Oxygen, Water, Ethanol, Hydrogen). Below these are checkboxes for 'Additional properties' (Binary diffusivities, Thermal conductivity, Viscosity, Fugacity coefficients, P1/P2 departure functions) and 'Output options' (Format: Text). A 'Calculate Real Gas Properties' button is at the bottom. On the right, the results panel displays: EOS: PR, Composition: $x_{CH_4} = 0.8$, $x_{CO_2} = 0.2$, $T = 200 \text{ }^\circ\text{C}$, $P = 100 \text{ bar}$, $Z = 0.986075$, Density = 56.0741 kg/m³, $\rho_{CH_4} = 0.981778$, $\rho_{CO_2} = 0.937953$, Gas viscosity = 1.85503e-05 Pa s, Thermal conductivity = 0.0585961 W/(m K). Buttons for 'Perform a new calculation', 'Reset form and restart', and 'Give feedback on this output' are at the bottom of the results panel.

- Online application
- Reads form data
- Processes inputs
- Calls executable
- Converts units
- Returns formatted results

<http://esdtools.lbl.gov/gaseos/>