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Risk Based Area of Review Delineation with MODFLOW and Groundwater Contaminant Fate and Transport Modeling

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Area of Review (AoR) delineation

- The AoR is the CO₂ plume and pressure zone that may risk Underground Source of Drinking Water (USDW).
- Defined by computational modeling, it covers the predicted maximum extent of the plume and/or pressure front over the project's lifetime.
- The pressure front is the pressure in the injection zone high enough to push fluids through a hypothetical conduit into an overlying USDW.





Source: EPA, 2013 after DBS&A



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General Steps for Risk Based AoR

- 1. Model brine leakage rates through a hypothetical improperly abandoned well at specified pressure increases within the injection zone.
- 2. Model the distribution of elevated salinity within the USDW resulting from leakage.
- 3. Compare estimated increase in USDW salinity to established screening levels and/or background values.
- 4. Map the maximum extent of the pressure front that impacts the USDW above screening levels and/or background levels.



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> Brine Borehole

Conceptual Model

- A single wellbore connects the injection zone to the USDW, dissipation zones, and shales.
- Dissipation zones receive most brine leakage due to proximity to injection zone.
- Shale zones are assumed impermeable outside of the wellbore.
- Salinity migrates with groundwater flow but a fraction also disperses upgradient.





Brine Leakage Modeling Approaches

- Approach 1: Hybrid Numerical and Analytical Modeling
 - Use MODFLOW to estimate brine flow and corresponding TDS flux rates from borehole to the dissipation zones and USDW.
 - Use analytical solutions to model fate and transport of TDS in the USDW from the borehole.
- Approach 2: Numerical Modeling
 - Use variable density, non-isothermal numerical model to model brine flow and fate and transport of TDS in the USDW.
- Both methods assume borehole is outside of CO₂ plume but within the area of increased pressure so that multiphase modeling is not required.



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Hunt/Wexler Analytical Solution

- Hunt (1978) solves the advection-dispersion equation with decay.
- Uses a point flux boundary.
- Wexler (1992) added sorption.
 - Sorption and decay can apply to other contaminants but not salinity.
- Assumes uniform flow, an infinite aquifer, and isothermal conditions.
 - Does not consider density-driven flow.

3D View of Hunt Analytical Solution with Grid for comparison





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Implementation of Hunt/Wexler

- Coded in MATLAB and Python.
- Uses superposition/image theory for boundary conditions and time-varying brine flux.
- Verified with MT3D.
- Compared to MODFLOW-SEAWAT for density-driven flow threshold.
 - Can be applied for brines < 15,000 mg/L TDS





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Approach 2 MODFLOW-SEAWAT Numerical Model

- Use MODFLOW-SEAWAT when density (>15,000 mg/L TDS) or non-isothermal effects impact brine flow.
- MODFLOW-SEAWAT integrates MODFLOW (flow) and MT3DMS (transport) for 3D variable-density simulation.
- Models heat transport, density changes from solute/temperature variations, and viscosity shifts due to temperature and salinity.



SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport



Techniques and Methods Book 6, Chapter A22

U.S. Department of the Interior U.S. Geological Survey



Key Input Parameters for Brine Leakage Modeling

- Stratigraphy
- Permeability of the USDW and Dissipation Zones
- Wellbore Permeability and Diameter
- Brine density and temperature
- Reservoir pressure at the wellbore
- Initial Total Dissolved Solids (TDS) for each formation
- Dispersivity



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Permeability of Borehole

- Open borehole permeability is often assumed to be ≤10⁻¹⁰ m² (101,325 mD), a conservative estimate exceeding reported values for leaking wells.
 - Celia et al. (2011) classify deep leakage potential from "low" to "extreme," with extreme cases ranging from 8 to 10,000 mD (8-x 10⁻¹⁵ to 1-x 10⁻¹¹ m²).
- Plugged wellbores are conservatively assumed to have a permeability of 10⁻¹³ m² (101 mD).

Table 2

Mapping of well score to mean effective well permeability. Data in columns marked with * from Watson and Bachu (2008).

Deep leakage potential*	Score range*	Well effective permeability mean [mD]
Low	<2	0.01-0.02
Medium	2-6	0.02-0.5
High	6-10	0.5-8
Extreme	>10	8-10,000

M.A. Celia et al. / International Journal of Greenhouse Gas Control 5 (2011) 257-269



Case Study

- Used Hybrid approach with MODFLOW and Hunt/Wexler.
- Model location with minimum distance between injection zone and USDW outside of CO₂ plume.
- Reservoir pressure set to constant 3,000 pounds per square inch (psi), which is 525 psi above hydrostatic conditions.
- MODFLOW simulations were conducted for 40 years, which is ten years longer than the planned injection timeframe.



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MODFLOW Grid and Conceptual Model



100 m x 100 m



Results



The predicted increase in TDS within USDWs, when averaged over the aquifer thickness, is expected to be less than 1 mg/L.



Interpretation Methods

- Method 1: Evaluate TDS concentration increase compared to regulatory groundwater quality standards.
- Method 2: Statistical analysis to evaluate TDS concentration increase compared to typical TDS variability in the USDW:
 - Method 2A: Comparison to typical well concentration fluctuation.
 - Method 2B: Comparison to Aquifer TDS Variability, Statistical Analysis (Last et al., 2016).



Method 1: Comparison to Water Quality Standards

- TDS has a recommended drinking-water secondary maximum contaminant (Secondary MCL) of 500 mg/L (22 CCR 64449).
 - Secondary MCLs are not health-based standards, but are guidelines for aesthetic considerations such as taste, color, and odor.
 - Site USDW already exceeds secondary MCL for TDS due to natural existing conditions.
- TDS tolerance levels for agriculture irrigation supply is generally less than 1,000 mg/L.
 - No predicted increase above 1,000 mg/L agricultural use limit beyond the plume footprint (215–230 mg/L increase).



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Method 2A: Comparison to Aquifer TDS Variability, Observed Fluctuation

- TDS fluctuates in local groundwater wells due to natural variability.
- 10-year TDS range (within 10 miles of injection site):
 - Average range: 131 mg/L
 - Maximum range: 700 mg/L
- Increase (<1 mg/L) is smaller than natural fluctuations and would be undetectable.





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Method 2B: Statistical Analysis

- Last et al. (2016) methodology for deriving groundwater threshold values.
- Median or average represents initial aquifer condition.
- Upper tolerance limit with 95 percent confidence and 95 percent coverage (UTL95-95) or 95 upper confidence limit (95-UCL) are upper end of background concentrations.
- Any TDS change from leakage, even under conservative assumptions, would be undetectable.



TDS Histogram, Median and 95-percent Upper Confidence Level



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Conclusions

- Risk-based AoR delineation provides a structured approach to evaluate potential groundwater impacts and is consistent with Class VI guidance.
- Hybrid numerical and analytical modeling effectively assesses brine leakage and contaminant transport where source TDS is less than 15,000 mg/L.
- Numerical modeling with MODFLOW-SEAWAT can be used to incorporate variable density and temperature effects in brine flow modeling for high TDS cases.
- Statistical methods help differentiate natural variability from potential project impacts.



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Questions?



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