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Sensitivity of thermal-hydrological-chemical simulations to choice of numerical algorithm

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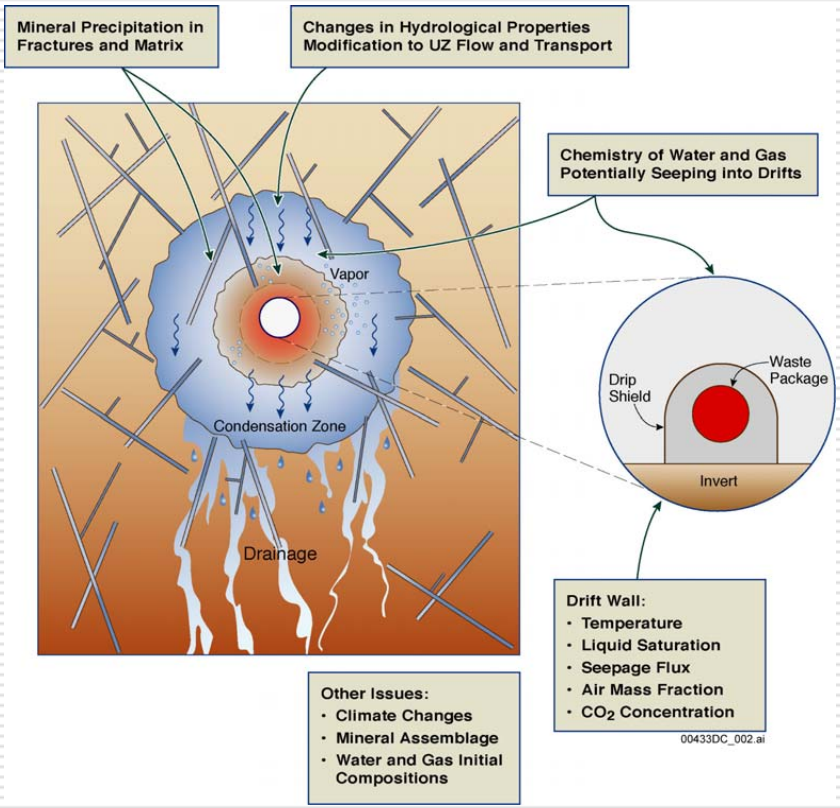
Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15–19, 2007

Thermal-hydrological-chemical (THC) simulations

- Used to investigate anticipated conditions in the host rock of the potential repository at Yucca Mountain, Nevada
  - Temperature, liquid content, humidity
  - Aqueous chemistry
  - Persistent changes in hydrological parameters
- Multiphysics codes
  - Two-phase porous media flow
  - Heat transport
  - Multicomponent reactive transport
  - Mineral precipitation and dissolution



Source: U.S. Department of Energy

Thermal-hydrological-chemical (THC) simulations – 2

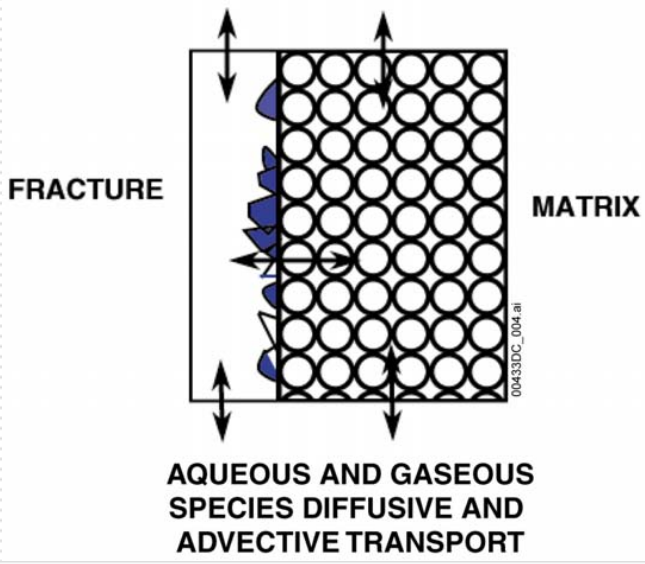
- Relatively few codes address above- boiling conditions
  - TOUGHREACT (Xu, et al., 2004)
  - MULTIFLO™ (Lichtner, 1996; Painter and Seth, 2003)
- Limited experience base for reactive transport near boiling regions
  - Numerical artifacts
  - Performance optimization

Objective

- Investigate various options for coupling chemical transport and reactions in strongly non-isothermal conditions
- Use MULTIFLO code and conditions expected in potential repository at Yucca Mountain
- Focus on mineralization patterns and chemistry of potential seepage water

MULTIFLO

- Developed by CNWRA for U.S. Nuclear Regulatory Commission
- Multiphysics
  - Two-phase (gas and liquid), two-component (air and H_2O) flow
  - Heat transport
  - Two-phase, multicomponent reactive transport
- Dual continuum (fracture and matrix) formulation
- Finite volume
  - Fully unstructured
  - Arbitrary (user specified) intercell connectivity
  - Hybrid upwind/central differencing
- Fully implicit with Newton iteration
- Iterative sparse solvers
  - Biconjugate Gradient Stabilized (BCGSTAB)
  - Preconditioning by incomplete lower-upper (ILU) with fixed level of fill



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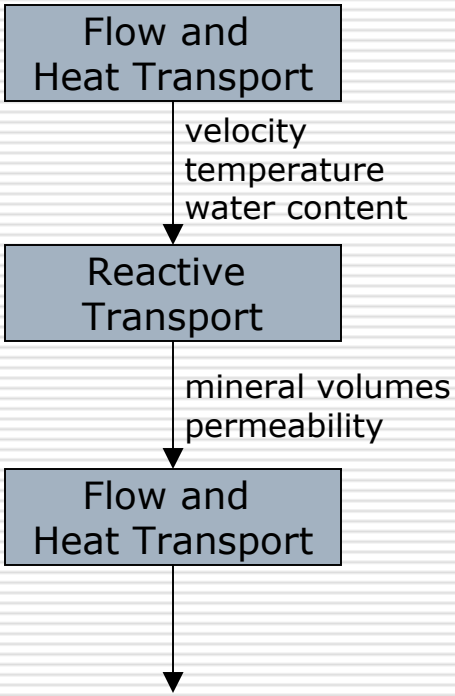
Process coupling in MULTIFLO

- Heat transport and flow are fully coupled
- Thermal hydrology and reactive chemical transport are sequential and non-iterative
- Multiple options for coupling reactions and chemical transport
  - Global implicit (slowest, most accurate)
  - Basic split operator
  - Strang splitting



Multicomponent, multiphase reactive transport

For j-th primary species $$\frac{\partial}{\partial t}\sum_{p=l,g}\phi s_p \Psi_{p,j} + \sum_{p=l,g} T_p \Psi_{p,j} = -\sum_m \nu_{jm} I_m$$

$\Psi_{p,j}$	Generalized concentration j-th species, p-th phase
T_p	Transport operator (advection and dispersion)
s_p	Phase saturation ($s_l + s_g = 1$)
I_m	Reaction rate for m-th mineral (function of concentrations)
ν_{jm}	Stoichiometric coefficient
ϕ	Porosity
t	Time

For m-th mineral $$\frac{\partial}{\partial t}\varphi_m = \overline{V}_m I_m$$

φ_m	Mineral abundance	$\overline{V}_m$	Mineral molar volume

Coupling reactions and transport

- Global implicit
  - Reaction and transport system solved iteratively as one big system
- Simple split operator
  - Transport with no reactions
  - Reactions using concentrations from transport substep
- Strang splitting
  - Transport half step
  - React
  - Transport half step

Simple split operator algorithm

Transport Step $$\frac{\partial}{\partial t}\sum_{p=l,g}\phi s_p \tilde{\Psi}_{p,j} + \sum_{p=l,g} T_p \tilde{\Psi}_{p,j} = 0$$

Reaction Step $$\frac{\partial}{\partial t}\sum_{p=l,g}\phi s_p \Psi_{p,j} = -\sum_m \nu_{jm} I_m$$

With initial condition from transport step $\Psi_{p,j}(\mathbf{r},t) = \tilde{\Psi}_{p,j}(\mathbf{r},t+\Delta t)$

Notes: Transport step decouples species

Reaction step decouples grid blocks

CPU and memory requirements greatly reduced

Variant of split operator algorithm

Fix reaction rate at beginning of transport step

$$\frac{\partial}{\partial t}\sum_{p=l,g}\phi s_p \tilde{\Psi}_{p,j} \quad + \quad \sum_{p=l,g} T_p \tilde{\Psi}_{p,j} \quad = \quad -w\sum_m \nu_{jm} I_m^0$$

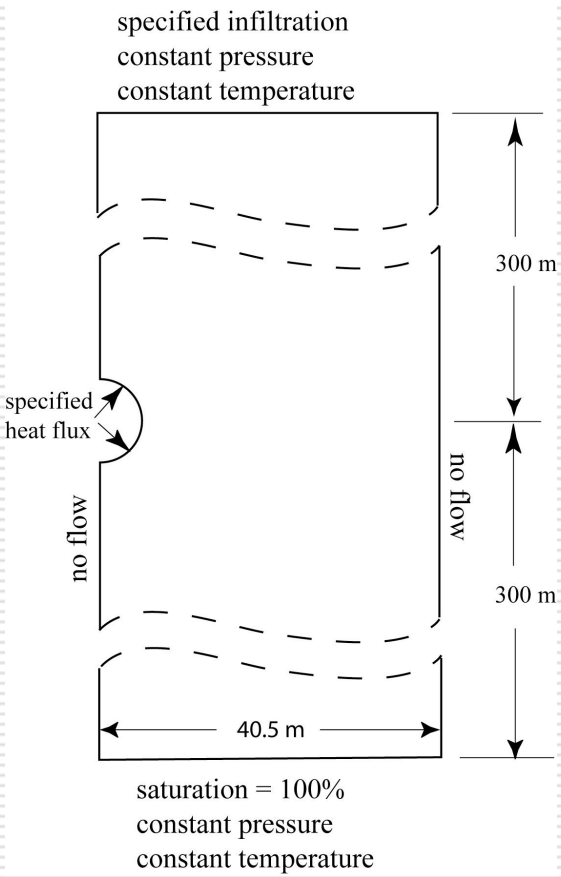
And remove from reaction step

$$\frac{\partial}{\partial t}\sum_{p=l,g}\phi s_p \Psi_{p,j} \quad = \quad -\sum_m \nu_{jm} I_m + w\sum_m \nu_{jm} I_m^0$$

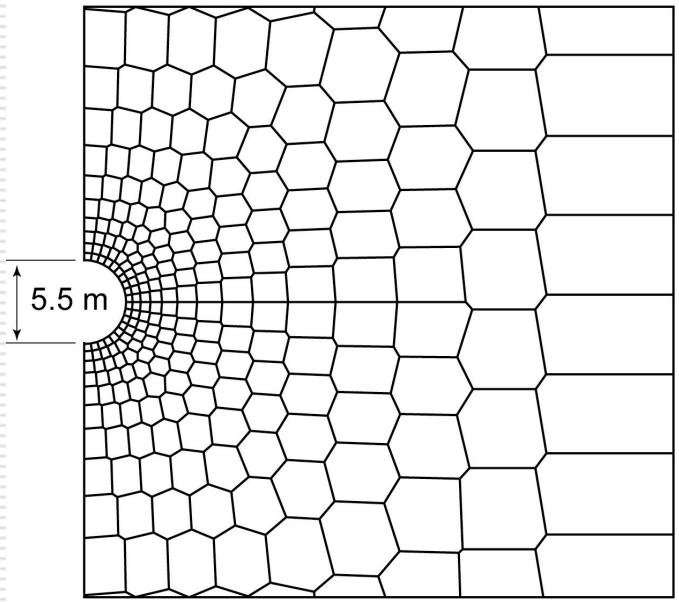
w is a weighting factor $0 \le w \le 1$

Initial tests show improved accuracy in isothermal conditions.

Test case grid



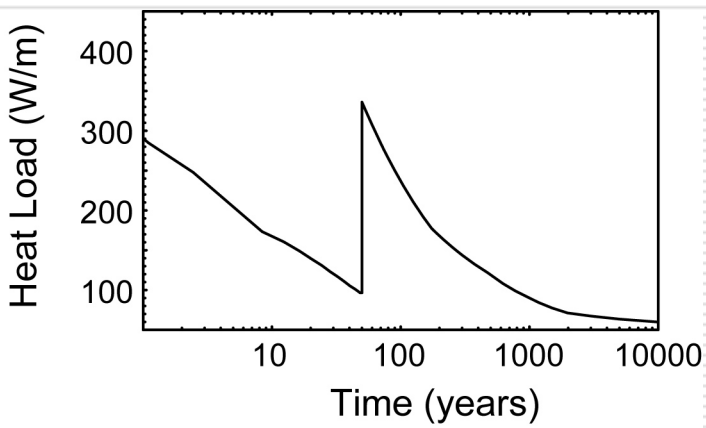
Detail from grid

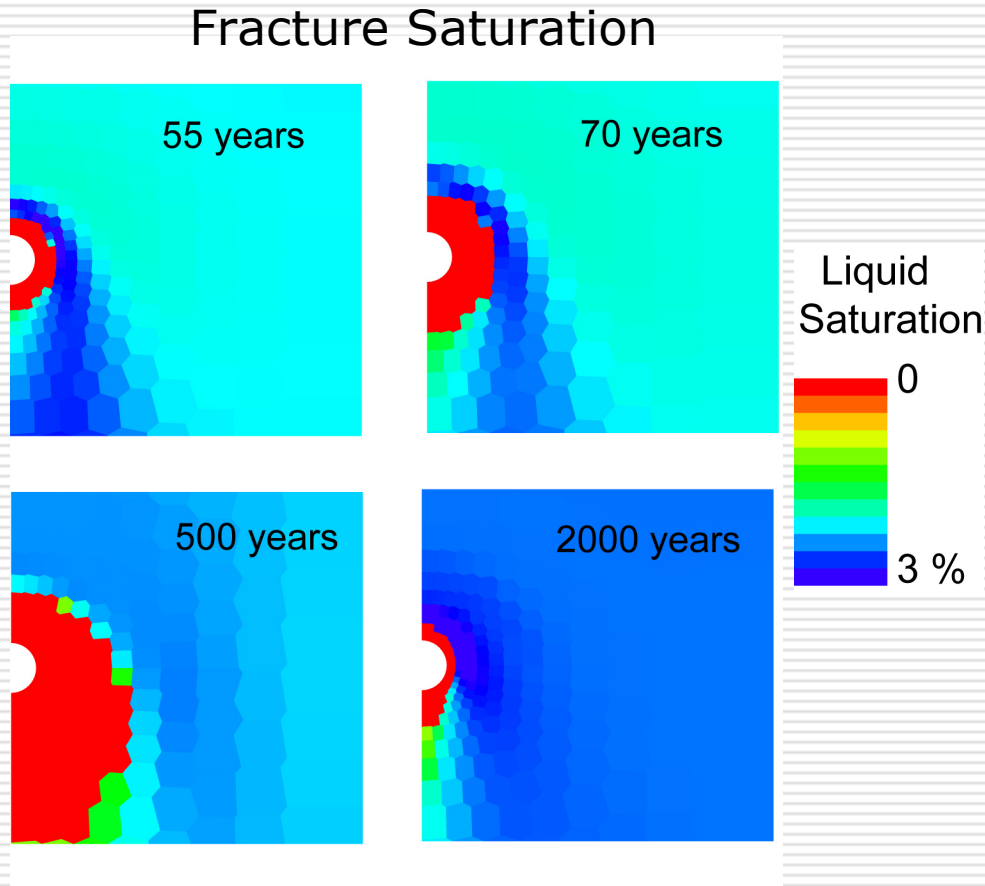


446 cells, dual continuum

Test case thermal hydrology

- Assumes forced ventilation ceases at t=50 years





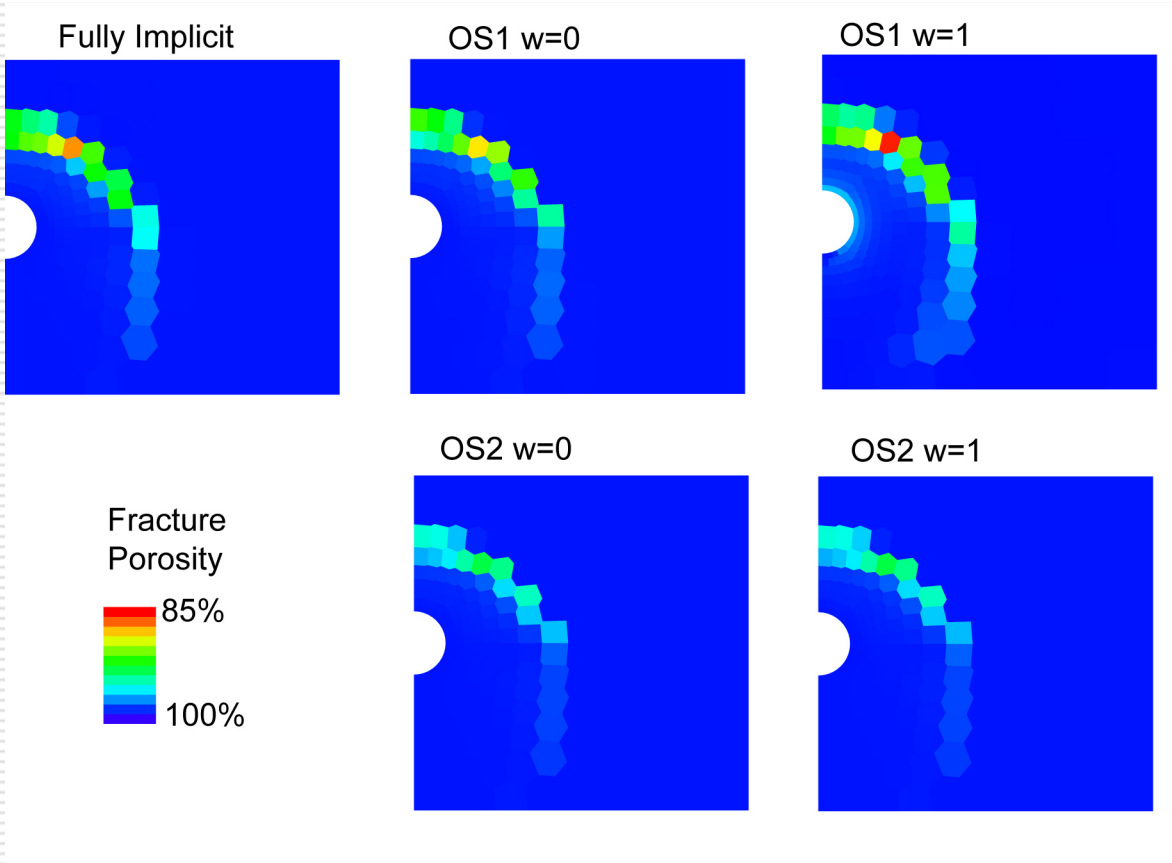
Test case geochemistry

- "Simplified" system of Spycher, et al. (2005)
- 21 aqueous species
- CO_2 gas
- 7 minerals
  - Calcite, fluorite, gypsum
  - Amorphous silica
  - Other silica phases (dissolution only)

Test cases

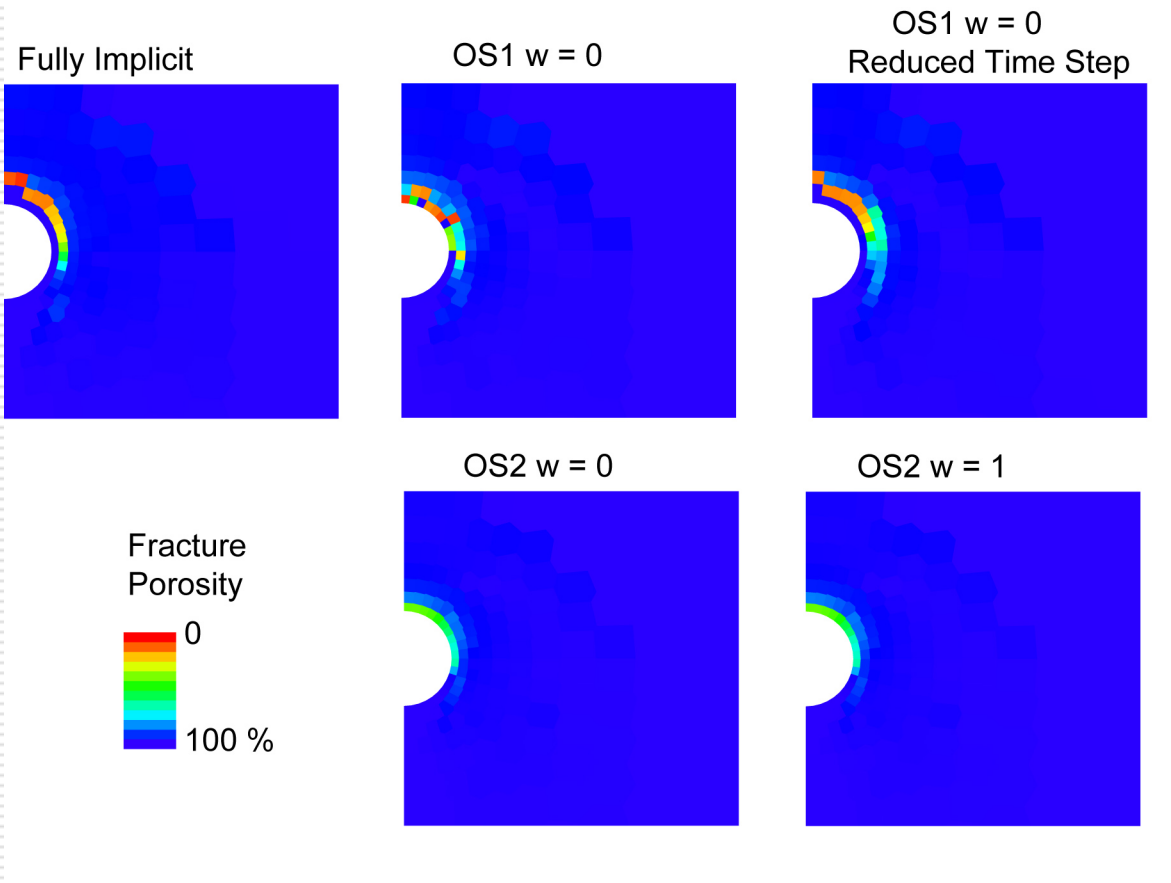
- FI: Fully implicit
- OS1: Single-step split operator
  - $w = 0,1/2,1$
- OS2: Strang splitting
  - $w = 0,1/2,1$

Fracture intrinsic porosity at 500 years



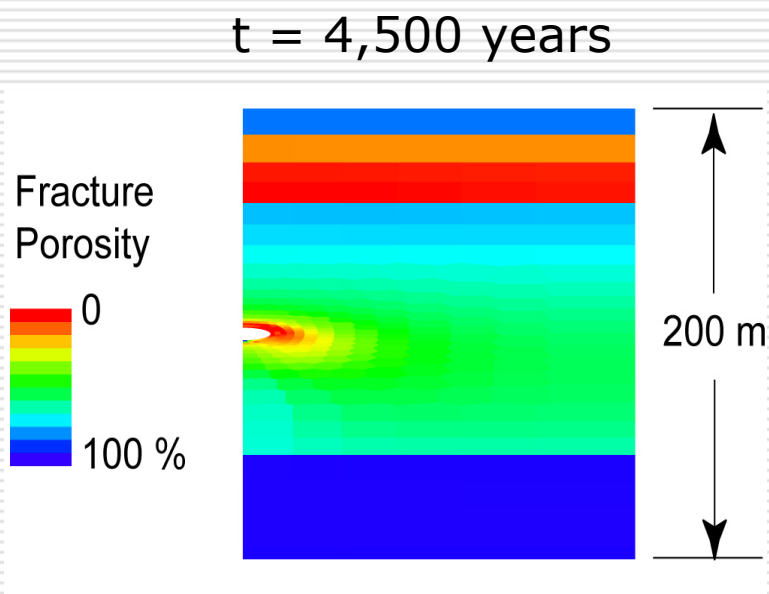
Note: An open fracture has intrinsic porosity of 100%

Fracture intrinsic porosity at 2,000 years

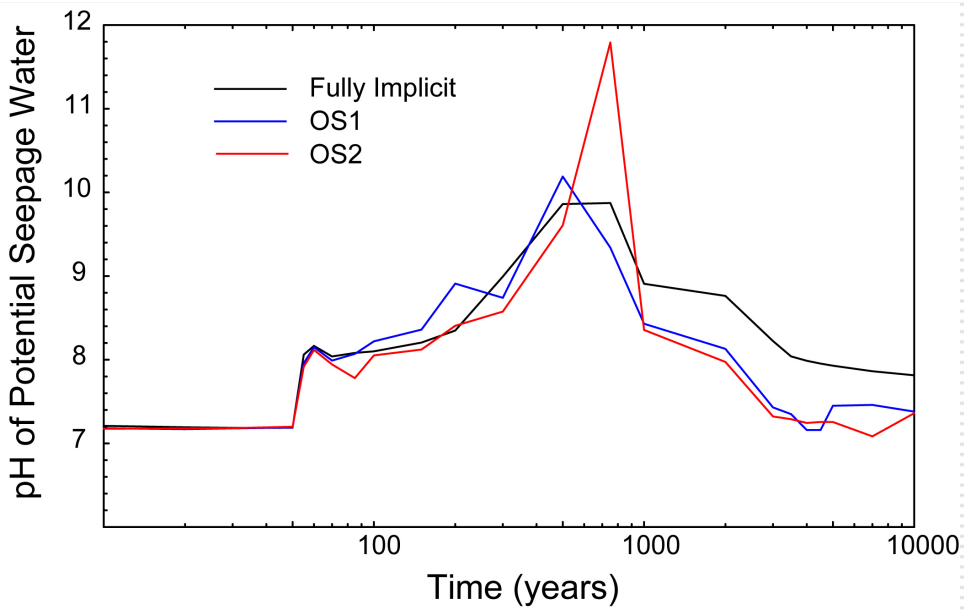


Numerical artifact with $w \neq 0$

- Adding initial reaction rate in transport step produced nonphysical result
  - Complete plugging of fractures by calcite above repository horizon
  - Only for OS1 and $w \neq 0$
  - Cause has not been identified



pH of potential seepage water



- Defined as pH in closest non-dry grid cell above tunnel crown

Run times

- For same time-step control parameters, split operator methods decreased run time by factor of ~3
- But, shorter time steps were required to match mineralization pattern at 2,000 years
- Net result was comparable run times

Summary of results

- For general mineralization pattern at 500 years, all split operator methods were consistent with the fully implicit results
- Simple splitting was best at matching the fully implicit results at 2,000 years, but required reduced time step that eliminated any advantage in run time
- Simple splitting was best at matching the fully implicit water chemistry results
- Incorporating initial reaction rate in transport step produced nonphysical result (t > 4,000 years) and generally yielded no improvement in accuracy
- Strang splitting resulted in no improvement over simple splitting

Conclusions

- For strongly nonisothermal systems that produce significant mineral precipitation, split operator methods offer little advantage in computational efficiency
- If conditions do not approach full plugging of fractures/pores, then split operator methods are viable alternatives to fully implicit
  - Approximate factor of 3 reduction in run time
- Simple (1-step) method was better than Strang splitting?
- Results of this study are different from experience with less reactive systems

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