Contract No:

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SRNL-STI-2017-00519

Date: August 14, 2017

To: Tom Butcher

From: Greg Flach

Reviewer: Larry Hamm

3.6 PORFLOW Code Improvements

Recommendation #136

Numerical Convergence Improvements for PORFLOW Unsaturated Flow Simulations

Scope Abstract: Section 3.6 of SRNL (2016) discusses various PORFLOW code improvements to increase modeling efficiency, in preparation for the next E-Area Performance Assessment (WSRC 2008) revision. This memorandum documents interaction with Analytic & Computational Research, Inc. (http://www.acricfd.com/default.htm) to improve numerical convergence efficiency using PORFLOW version 6.42 for unsaturated flow simulations.

Results / Conclusions: A 10x reduction in simulation time has been achieved for a challenging simulation problem by using a more efficient PORFLOW solver and optimized relaxation scheme.

Discussion:

Simulation of unsaturated porous medium flow is well known to be challenging because of strong nonlinearity introduced by moisture characteristic curves. Figure 1 illustrates a particularly difficult simulation problem taken from the H-Tank Farm (HTF) Performance Assessment (PA). The simulation involves a concrete tank filled with grout. The geometry is a 2D radial cut reflecting axisymmetric conditions (Figure 1a). Cementitious materials are physically degraded (cracked/fractured) but still lower permeability than surrounding soil. Characteristic curves are a blend or composite of two materials (Figure 1b):

- low-permeability / high air-entry pressure material representing the intact portion (matrix)
- high-permeability / low air-entry pressure material representing fractures/cracks

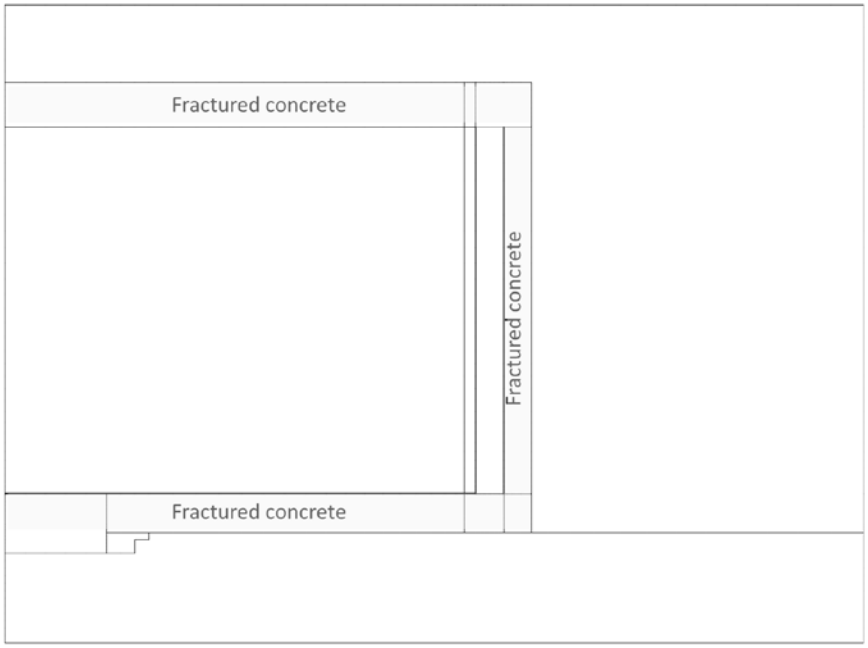
Infiltration descends down from upper surface, then around and underneath tank (Figure 2). The water table coincides with lower boundary, and no flow crosses the left (centerline) or right sides.

Table 1 presents PORFLOW settings that have typically been used in the HTF PA, and Figure 3 illustrates PORFLOW simulation results. “Saturation discrepancy” is saturation computed from PORFLOW pressure head (“P”) and the material characteristic curve, minus saturation reported by PORFLOW. Saturation discrepancy occurs when PORFLOW saturation (“S”) is relaxed during numerical simulations to dampen numerical oscillations, such that P and S are no longer precisely linked through the characteristic curve. Both the mass balance and saturation discrepancies are acceptably small in Figure 3b, however, the simulation wall-clock time was approximately 100 minutes, which is longer than desired.

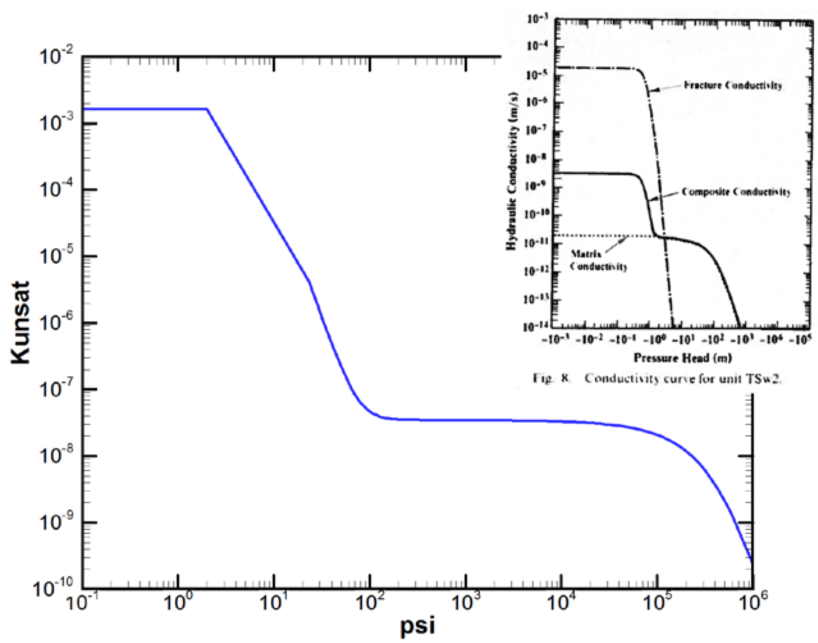
Table 2 presents more efficient PORFLOW settings, and Figure 4 shows the simulation results. The simulation time is about 10 minutes, or 10x faster than the reference case. The saturation discrepancy is also lower than that of the reference case. Most of the speedup comes from switching from the direct LUDE solver to an iterative CONJugate gradient with CHOLesky preconditioner solver. Some numerical efficiency and the improved saturation convergence are achieved by smoothly decreasing the saturation relaxation factor in a geometric manner.

Through saturation RELAxation = 0.01, the number of iterations increases geometrically starting from a reference value of 10, subject to a minimum of 50. The first phase, or left hand column of Table 2, is designed to slowly dampen numerical instabilities while allowing an adequate number of iterations for the simulation to migrate from the initial conditions (full saturation) to the neighborhood of the converged solution. Beyond RELAxation = 0.01 (right hand column of Table 2) the primary objective is to eliminate numerical noise. 400 iterations are uniformly specified in this second phase.

The settings in Table 2 are thought to be robust, that is, they are expected to generally perform well for other challenging flow simulations.



(a)



(b)

Figure 1. Test problem selected from H-Tank Farm PA: (a) geometry and key attributes, (b) material properties of fractured concrete.

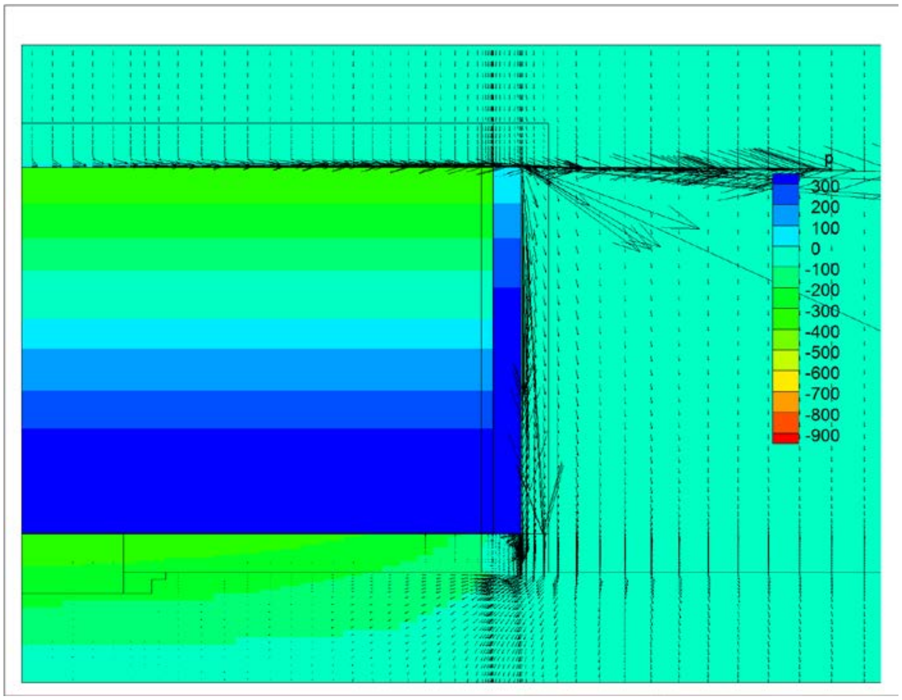


Figure 2. PORFLOW flow simulation.

Table 1. Reference PORFLOW settings reflecting typical SRNL practice.

```
PROPerty P UPWI
MATRix LUDE for P
CONVergence for P    1.e-6, 1 iterations max
SET P to: 0

!!Migrate to solution neighborhood
SOLVe STEAdy 50
RELAx S 0.7
SOLVe STEAdy 50
RELAx S 0.3
SOLVe STEAdy 150
RELAx S 0.1
SOLVe STEAdy 450

!!Mixed purpose
RELAx S 0.03
SOLVe STEAdy 1500
RELAx S 0.01
SOLVe STEAdy 1500

!!Suppress noise / sharpen mass balance
RELAx S 0.003
SOLVe STEAdy 2000
RELAx S 0.001
SOLVe STEAdy 2000
RELAx S 0.0003
SOLVe STEAdy 2000
RELAx S 0.0001
SOLVe STEAdy 2000
RELAx S 0.00001
SOLVe STEAdy 2000
RELAx S 0.000001
SOLVe STEAdy 2000
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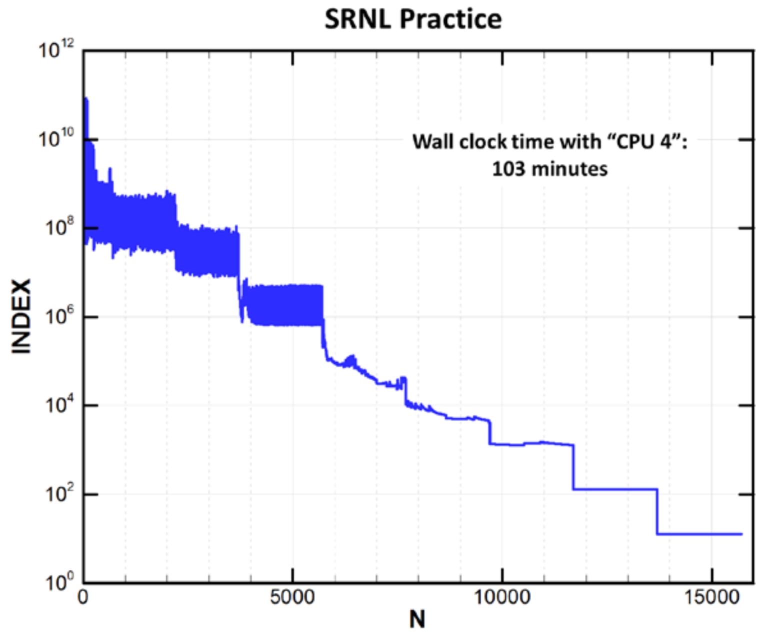
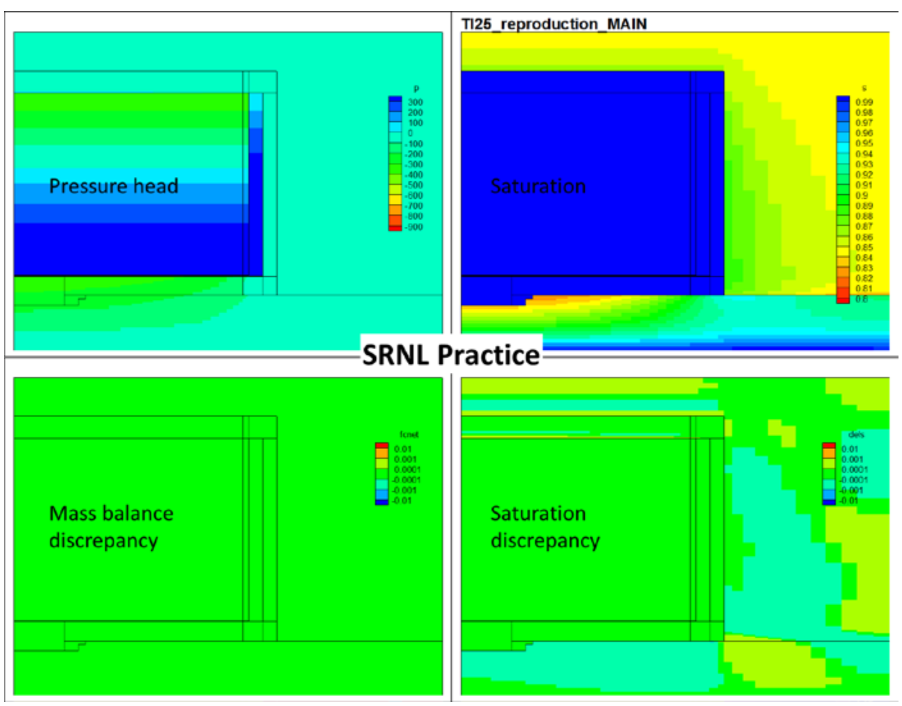


(a)



(b)

Figure 3. PORFLOW flow simulation using reference settings (Table 1): (a) convergence history, and (b) simulated flow field and numerical balances.

Table 2. Improved PORFLOW settings.

```
PROPerty P UPWI
MATRix for P CHOL CONJ
MATRix ITERation 100
CONVergence for P    1.e-12, 1 iterations max
SET P to: 0

SOLVe STEAdy 50
SAVE P S U V MOIS FC to "01.sav" NOW

RELAxation for S 7.94E-01; SOLVe STEAdy 50
RELAxation for S 6.31E-01; SOLVe STEAdy 50
RELAxation for S 5.01E-01; SOLVe STEAdy 50
RELAxation for S 3.98E-01; SOLVe STEAdy 50
RELAxation for S 3.16E-01; SOLVe STEAdy 50
SAVE P S U V MOIS FC to "02.sav" NOW

RELAxation for S 2.51E-01; SOLVe STEAdy 50
RELAxation for S 2.00E-01; SOLVe STEAdy 50
RELAxation for S 1.58E-01; SOLVe STEAdy 63
RELAxation for S 1.26E-01; SOLVe STEAdy 79
RELAxation for S 1.00E-01; SOLVe STEAdy 100
SAVE P S U V MOIS FC to "03.sav" NOW

RELAxation for S 7.94E-02; SOLVe STEAdy 126
RELAxation for S 6.31E-02; SOLVe STEAdy 158
RELAxation for S 5.01E-02; SOLVe STEAdy 200
RELAxation for S 3.98E-02; SOLVe STEAdy 251
RELAxation for S 3.16E-02; SOLVe STEAdy 316
SAVE P S U V MOIS FC to "04.sav" NOW

RELAxation for S 2.51E-02; SOLVe STEAdy 398
RELAxation for S 2.00E-02; SOLVe STEAdy 501
RELAxation for S 1.58E-02; SOLVe STEAdy 631
RELAxation for S 1.26E-02; SOLVe STEAdy 794
RELAxation for S 1.00E-02; SOLVe STEAdy 1000
SAVE P S U V MOIS FC to "05.sav" NOW
```

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(continued from adjacent column)

RELAxation for S 7.94E-03; SOLVe STEAdy 400
RELAxation for S 6.31E-03; SOLVe STEAdy 400
RELAxation for S 5.01E-03; SOLVe STEAdy 400
RELAxation for S 3.98E-03; SOLVe STEAdy 400
RELAxation for S 3.16E-03; SOLVe STEAdy 400
SAVE P S U V MOIS FC to "06.sav" NOW

RELAxation for S 2.51E-03; SOLVe STEAdy 400
RELAxation for S 2.00E-03; SOLVe STEAdy 400
RELAxation for S 1.58E-03; SOLVe STEAdy 400
RELAxation for S 1.26E-03; SOLVe STEAdy 400
RELAxation for S 1.00E-03; SOLVe STEAdy 400
SAVE P S U V MOIS FC to "07.sav" NOW

RELAxation for S 7.94E-04; SOLVe STEAdy 400
RELAxation for S 6.31E-04; SOLVe STEAdy 400
RELAxation for S 5.01E-04; SOLVe STEAdy 400
RELAxation for S 3.98E-04; SOLVe STEAdy 400
RELAxation for S 3.16E-04; SOLVe STEAdy 400
SAVE P S U V MOIS FC to "08.sav" NOW

RELAxation for S 2.51E-04; SOLVe STEAdy 400
RELAxation for S 2.00E-04; SOLVe STEAdy 400
RELAxation for S 1.58E-04; SOLVe STEAdy 400
RELAxation for S 1.26E-04; SOLVe STEAdy 400
RELAxation for S 1.00E-04; SOLVe STEAdy 400
SAVE P S U V MOIS FC to "09.sav" NOW

RELAxation for S 1.00E-06; SOLVe STEAdy 400
SAVE P S U V MOIS FC to "10.sav" NOW
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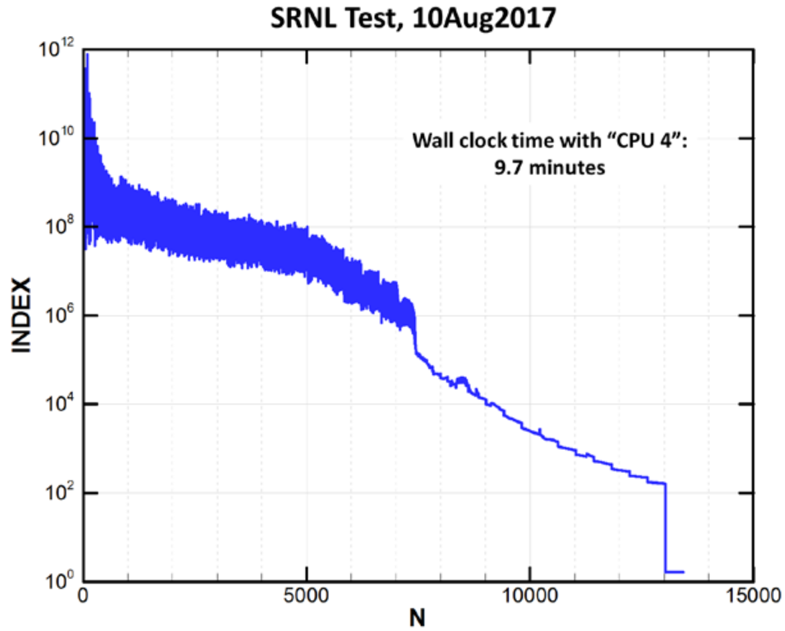
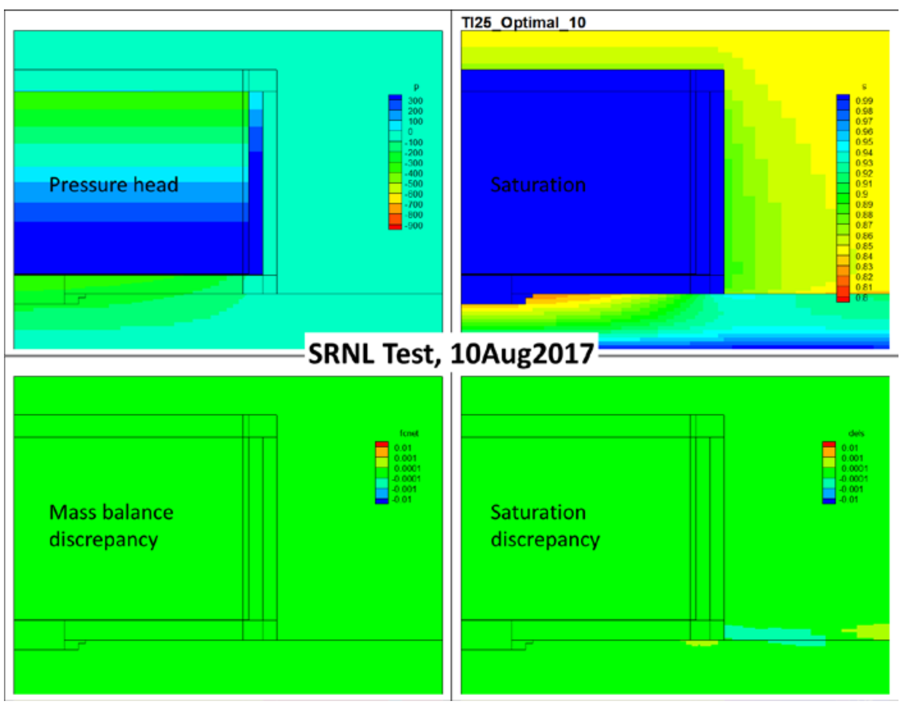


(a)



(b)

Figure 4. PORFLOW flow simulation using the improved settings (Table 2): (a) convergence history, and (b) simulated flow field and numerical balances.

<u>References</u>:

SRNL. *Strategic Plan for Next E-Area Low-Level Waste Facility Performance Assessment. Appendix 1.0, Topical Presentations and Team Deliberations*. SRNL-STI-2015-00620 Revision 0. February 2016.

Washington Savannah River Company LLC. *E-Area Low-Level Waste Facility DOE 435.1 Performance Assessment*. WSRC-STI-2007-00306, Revision 0. July 2008.

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