Problem Description of Modeling a Leak from the SX-115 Tank at the Hanford S/SX Tank Farm

P.C. Lichtner

February 21, 2011

Problem Description

The saturation profile is computed for both steady-state and transient conditions in a 1D vertical column consisting of a layered porous medium representing the Hanford sediment in the vicinity of the S/SX tank farm. The transient case simulates a leak from the base of the SX-115 tank. This problem description is taken from Lichtner et al. (2004).

Governing Equations

The moisture profile is calculated using parameters related to the Hanford sediment at the S/SX tank farm based on the Richards equation for variably saturated porous media. The Hanford sediment is composed of five layers with the properties listed in Tables 1 and 2. The governing equations consist of Richards equation for variably saturated fluid flow given by

$$\frac{\partial}{\partial t}\varphi s \rho + \boldsymbol{\nabla}\cdot \boldsymbol{q}\rho \;=\; Q, \tag{1}$$

and solute transport of a tracer

$$\frac{\partial}{\partial t}\varphi C + \boldsymbol{\nabla}\cdot \big(\boldsymbol{q}C - \varphi s \tau D \boldsymbol{\nabla} C\big) \;=\; Q_C. \tag{2}$$

In these equations φ denotes the spatially variable porosity of the porous medium assumed to constant within each stratigraphic layer, s gives the saturation state of the porous medium, ρ represents the fluid density in general a function of pressure and temperature, C denotes the solute concentration, D denotes the diffusion/dispersion coefficient, τ represents tortuosity, Q and Q_C denote source/sink terms, and $\boldsymbol{q}$ denotes the Darcy velocity defined by

$$\boldsymbol{q} \;=\; -\frac{k_{\rm sat}k_r}{\mu}\boldsymbol{\nabla}(p-\rho g z), \tag{3}$$

with saturated permeability $k_{\rm sat}$, relative permeability k_r, fluid viscosity μ, pressure p, formula weight of water W, acceleration of gravity g, and height z. Van Genuchten capillary properties are used for relative relative permeability according to the relation

$$k_r \;=\; \sqrt{s_{\rm eff}}\left\{1-\left[\left(s_l^{\rm eff}\right)^{1/m}\right]^m\right\}^2, \tag{4}$$

where $s_{\rm eff}$ is related to capillary pressure P_c by the equation

$$s_{\rm eff} \;=\; \left[1+(\alpha|P_c|)^n\right]^{-m}, \tag{5}$$

where $s_{\rm eff}$ is defined by

$$s_{\rm eff} \;=\; \frac{s-s_r}{1-s_r}, \tag{6}$$

and where s_r denotes the residual saturation. The quantity n is related to m by the expression

$$m \;=\; 1-\frac{1}{n}, \quad n \;=\; \frac{1}{1-m}. \tag{7}$$

The capillary pressure P_c and fluid pressure p are related by the (constant) gas pressure p_g^0

$$P_c \;=\; p_g^0 - p, \tag{8}$$

where $p_g^0 = 101,325$ Pa is set to atmospheric pressure.

Semi-Analytical Solution for Steady-State Conditions

For steady-state conditions the saturation profile satisfies the equation

$$\frac{d}{dz}\rho q_z \;=\; 0, \tag{9}$$

or assuming an incompressible fluid

$$q_z \;=\; q_z^0, \tag{10}$$

where q_z^0 denotes infiltration at the surface. Thus the pressure is obtained as a function of z by solving the ODE

$$\frac{dp}{dz} \;=\; -\frac{\mu q_z^0}{k_{\rm sat}k_r} - \rho g, \tag{11}$$

using Eqns.(4) and (5) to express the relative permeability k_r as a function of pressure. For the special case of zero infiltration it follows that

$$p(z) \;=\; p_0 - \rho g(z - z_0), \tag{12}$$

with $p(z_0) = p_0$. The saturation profile is obtained from Eqns.(5) and (6).

Model Parameters

Model parameters used in the simulations are listed in Tables 1 and 2. Although not needed here, thermal properties are also listed. Diffusivity was set to 10^{-9} m^2 s^{-1} and tortuosity was set to one.

Table 1: Stratigraphic sequence used in the calculations, after Ward et al. (1996).

Formation	Abbrev.	Thickness [m]
Backfill	BF	16.0
Hanford Fine Sand	HF	23.0
Plio-Pleistocene	PP	6.0
Upper Ringold Gravel	URG	3.0
Middle Ringold Gravel	MRG	20.0

Table 2: Parameters for material and thermal properties for intrinsic rock density ρ_s, heat capacity c, thermal conductivity κ, porosity φ, residual water saturation s_r, van Genuchten parameters α and λ, and vertical water saturated permeability $k_{\rm sat}$. Data taken from Khaleel and Freeman (1995), Khaleel et al. (2001), and Pruess et al. (2002).

Formation	ρ_s	c	$\kappa_{\rm dry}$	$\kappa_{\rm wet}$	φ	s_r	α	m	$k_{\rm sat}$
	g cm^{-3}	J kg^{-1} K^{-1}	W m^{-1}		—	—	m^{-1}	—	m^2
BF	2.8	800	0.5	2	0.2585	0.0774	1.008e-3	0.658	1.24e-12
HF	2.8	800	0.5	2	0.3586	0.0837	9.390e-5	0.469	1.23e-13
PP	2.8	800	0.5	2	0.4223	0.2595	6.840e-5	0.456	1.37e-14
URG	2.8	800	0.5	2	0.2625	0.2130	2.961e-5	0.386	5.27e-14
MRG	2.8	800	0.5	2	0.1643	0.0609	6.330e-5	0.392	7.33e-14

Simulation Results

The calculations are carried out for an isothermal system using Richards equation. First, the steady-state saturation profile is obtained without the tank leak present. Then using the steady-state profile as the initial condition the tank leak is turned on. The results for the steady-state saturation and pressure profiles are shown in Figure 1 for infiltration rates at the surface of 0, 8 and 80 mm/y. The mean infiltration rate at the Hanford site is approximately 8 mm/y. A 1D column 68 m heigh with the water table located at a height of 6 m from the bottom is used in the simulation. A uniform grid spacing of 0.5 m is used to discretize Richards equation.

Shown in Figure 2 is the saturation at different times following a two week leak releasing 60,000 gallons from the SX-115 tank at a depth of 16 m. In the simulation a release rate of 1.87×10^{-3} kg/s is used.

References

Khaleel, R., E.J. Freeman (1995) Variability and scaling of hydraulic properties for 200 area soils, Hanford Site. Report WHC-EP-0883. Westinghouse Hanford Company, Richland, WA.

Khaleel, R., T.E. Jones, A.J. Knepp, F.M. Mann, D.A. Myers, P.M. Rogers, R.J. Serne, and M.I. Wood (2000) Modeling data package for S-SX Field Investigation Report (FIR). Report RPP-6296, Rev. 0. CH2M Hill Hanford Group, Richland, WA.

Lichtner, P.C., Yabusaki, S.B., Pruess K., and Steefel, C.I. (2004) Role of Competitive Cation Exchange on Chromatographic Displacement of Cesium in the Vadose Zone Beneath the Hanford S/SX Tank Farm, *VJZ*, **3**, 203–219.

Pruess, K., S. Yabusaki, C. Steefel, and P. Lichtner (2002) Fluid flow, heat transfer, and solute transport at nuclear waste storage tanks in the Hanford vadose zone. Available at www.vadosezonejournal.org. Vadose Zone J. 1:68–88.

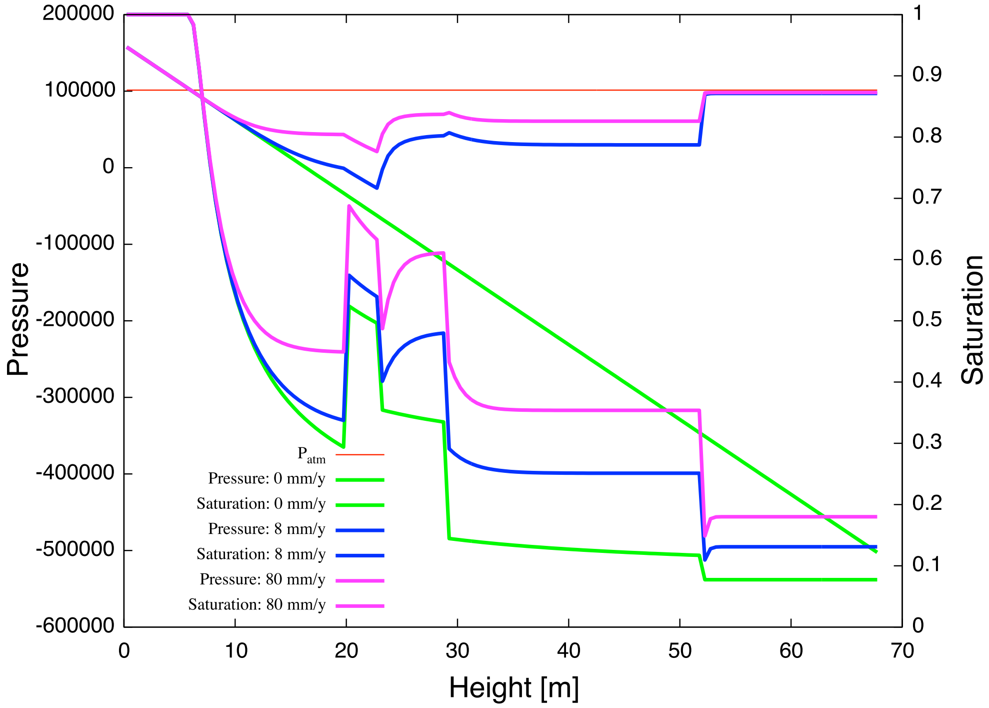

Figure 1: Steady-state saturation and pressure profiles for infiltration rates of 0, 8 and 80 mm/y. The water table is located at 6 m from the bottom of the computational domain.

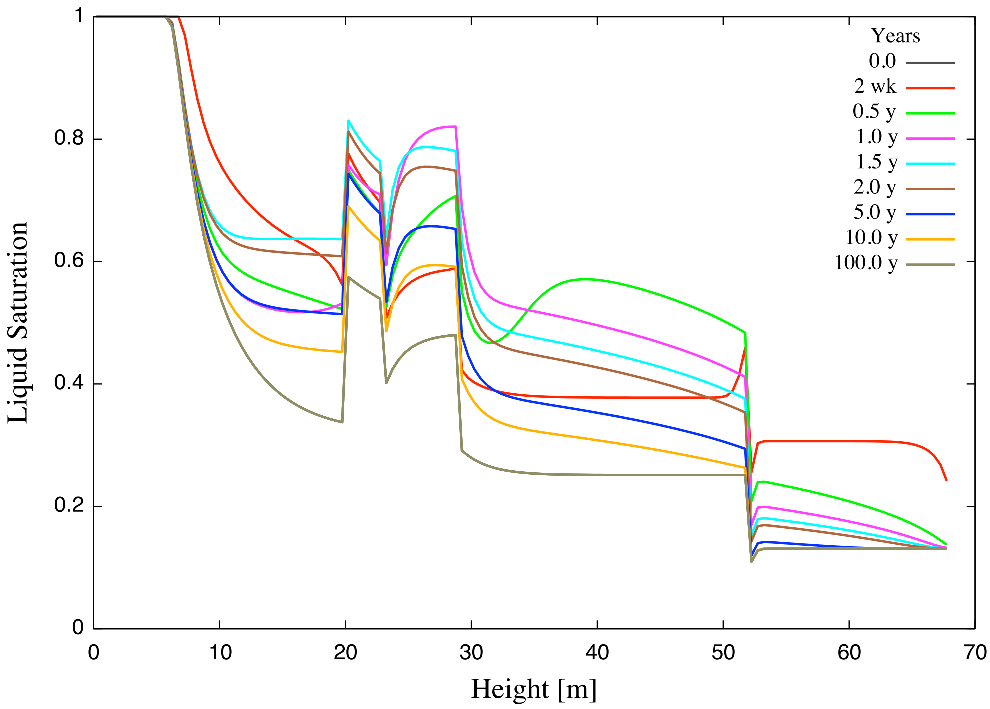

Figure 2: Simulation of a tank leak with a duration of two weeks showing the saturation profile for different times indicated in the figure.

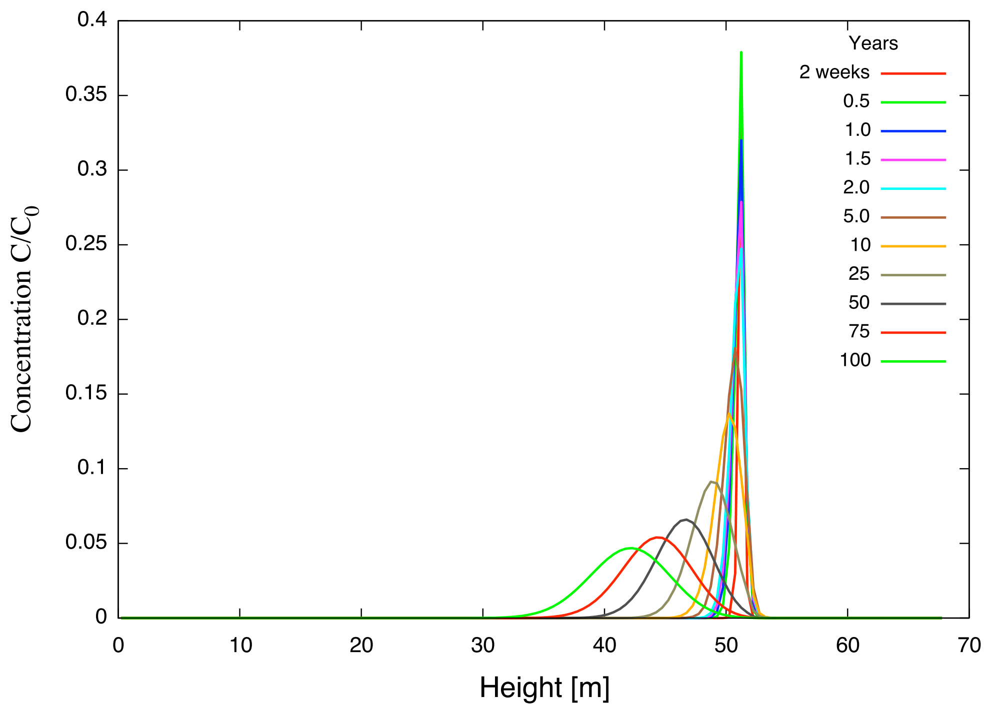

Figure 3: The solute concentration profile corresponding to Figure 2 for different times indicated in the figure.

PFLOTRAN Input Files

Listing of PFLOTRAN input file including a tracer. Note that the stratigraphic zone specification in `REGION` is grid independent as is the grid size specification in keyword `GRID`. Therefore to change the grid spacing only the line: `NXYZ 1 1 136`, needs to be changed. Also note that a line beginning with a colon (:) is read as a comment.

PFLOTRAN input file `pflotran.in`:

```
:Description: 1D infiltration problem for the SX-115 tank at Hanford

: == debugging =================================================================
DEBUG
:MATVIEW_JACOBIAN
:VECVIEW_RESIDUAL
:VECVIEW_SOLUTION
/

: == mode ======================================================================
MODE RICHARDS

:================ runtime ===================
CHECKPOINT 100000
RESTART restart.chk 0.d0

: == chemistry =================================================================
CHEMISTRY
PRIMARY_SPECIES
Tracer
/
OUTPUT
All
/
/

: == reference variables =======================================================
REFERENCE_POROSITY 0.25d0

: == time stepping =============================================================
TIMESTEPPER
TS_ACCELERATION 8
/

: == discretization ============================================================
GRID
TYPE structured
NXYZ 1 1 136
:DXYZ
:1.
:1.
:0.5
:/
BOUNDS
0.d0 1.d0
0.d0 1.d0
0.d0 68.d0
/
/

: == flow solvers ==============================================================
```

```
NEWTON_SOLVER FLOW
PRECONDITIONER_MATRIX_TYPE AIJ
RTOL 1.d-8
ATOL 1.d-8
STOL 1.d-30
ITOL_UPDATE 1.d0
:NO_INFINITY_NORM
:NO_PRINT_CONVERGENCE
:PRINT_DETAILED_CONVERGENCE
/

LINEAR_SOLVER FLOW
:KSP_TYPE FGMRES
:KSP_TYPE PREONLY
:PC_TYPE LU
/

: == transport solvers =========================================================
NEWTON_SOLVER TRANSPORT
PRECONDITIONER_MATRIX_TYPE AIJ
RTOL 1.d-12
ATOL 1.d-12
STOL 1.d-30
:NO_INFINITY_NORM
:NO_PRINT_CONVERGENCE
:PRINT_DETAILED_CONVERGENCE
/

LINEAR_SOLVER TRANSPORT
:KSP_TYPE PREONLY
:PC_TYPE LU
/

: == fluid properties ==========================================================
FLUID_PROPERTY
DIFFUSION_COEFFICIENT 1.d-9
/

: == material properties =======================================================
MATERIAL_PROPERTY BF
ID 1
SATURATION_FUNCTION BF
POROSITY 0.2585
TORTUOSITY 1.0
PERMEABILITY
PERM_ISO 1.24e-12
/
/

MATERIAL_PROPERTY HF
ID 2
SATURATION_FUNCTION HF
POROSITY 0.3586
TORTUOSITY 1.0
PERMEABILITY
PERM_ISO 3.37028e-13
/
/

MATERIAL_PROPERTY PP
ID 3
SATURATION_FUNCTION PP
POROSITY 0.4223
TORTUOSITY 1.0
PERMEABILITY
```

```
PERM_ISO 3.73463e-14
/
/

MATERIAL_PROPERTY URG
ID 4
SATURATION_FUNCTION URG
POROSITY 0.2625
TORTUOSITY 1.0
PERMEABILITY
PERM_ISO 1.4392e-13
/
/

MATERIAL_PROPERTY MRG
ID 5
SATURATION_FUNCTION MRG
POROSITY 0.1643
TORTUOSITY 1.0
PERMEABILITY
PERM_ISO 2.00395e-13
/
/

: == saturation / permeability functions ======================================
SATURATION_FUNCTION BF
SATURATION_FUNCTION_TYPE VAN_GENUCHTEN
RESIDUAL_SATURATION 0.0774
LAMBDA 0.6585
ALPHA 1.008d-3
/

SATURATION_FUNCTION HF
SATURATION_FUNCTION_TYPE VAN_GENUCHTEN
RESIDUAL_SATURATION 0.08366
LAMBDA 0.46944
ALPHA 9.40796e-5
/

SATURATION_FUNCTION PP
SATURATION_FUNCTION_TYPE VAN_GENUCHTEN
RESIDUAL_SATURATION 0.25953
LAMBDA 0.45587
ALPHA 6.85145e-5
/

SATURATION_FUNCTION URG
SATURATION_FUNCTION_TYPE VAN_GENUCHTEN
RESIDUAL_SATURATION 0.21295
LAMBDA 0.38594
ALPHA 2.96555e-5
/

SATURATION_FUNCTION MRG
SATURATION_FUNCTION_TYPE VAN_GENUCHTEN
RESIDUAL_SATURATION 0.06086
LAMBDA 0.39215
ALPHA 6.34015e-5
/

: == output ====================================================================
OUTPUT
:PERIODIC TIMESTEP 1
:PERIODIC TIME 0.025 y
times y 1. 10. 100.
```

```
FORMAT TECPLOT POINT
FORMAT HDF5
/

: == times ===================================================================
TIME
FINAL_TIME 100. y
INITIAL_TIMESTEP_SIZE 1.e-6 y
MAXIMUM_TIMESTEP_SIZE 1.e-1 y
/

: == regions =================================================================
REGION all
:BLOCK 1 1 1 1 1 136
COORDINATES
0.d0 0.d0 0.d0
1.d0 1.d0 68.d0
/
/
REGION Top
:BLOCK 1 1 1 1 136 136
FACE TOP
COORDINATES
0.d0 0.d0 68.d0
1.d0 1.d0 68.d0
/
/
REGION Bottom
:BLOCK 1 1 1 1 1 1
FACE BOTTOM
COORDINATES
0.d0 0.d0 0.d0
1.d0 1.d0 0.d0
/
/
REGION BF
:BLOCK 1 1 1 1 105 136
COORDINATES
0.d0 0.d0 52.d0
1.d0 1.d0 68.d0
/
/
REGION HF
:BLOCK 1 1 1 1 59 104
COORDINATES
0.d0 0.d0 29.d0
1.d0 1.d0 52.d0
/
/
REGION PP
:BLOCK 1 1 1 1 47 58
COORDINATES
0.d0 0.d0 23.d0
1.d0 1.d0 29.d0
/
/
REGION URG
:BLOCK 1 1 1 1 41 46
COORDINATES
0.d0 0.d0 20.d0
1.d0 1.d0 23.d0
/
/
REGION MRG
:BLOCK 1 1 1 1 1 40
```

```
COORDINATES
0.d0 0.d0 0.d0
1.d0 1.d0 20.d0
/
/
REGION Leak
:BLOCK 1 1 1 1 103 103
COORDINATES
0.d0 0.d0 51.d0
1.d0 1.d0 51.d0
/
/

: == flow conditions ==========================================================
FLOW_CONDITION Inlet
TYPE
FLUX neumann
/
:FLUX 3.17098d-10 ! 1 cm/y
:FLUX 1.5855d-10 ! 5 mm/y
FLUX 2.53678e-10 ![m/s] (8 mm/y)
:FLUX 0.d0
:FLUX file 200w_recharge_1951-2000_daily.dat
/

FLOW_CONDITION Initial
TYPE
PRESSURE hydrostatic
/
DATUM 0.d0 0.d0 6.d0
PRESSURE 101325.d0
/

skip
FLOW_CONDITION source
TYPE
RATE mass_rate
/
INTERPOLATION STEP
RATE file src.dat ! 8.4e-4 kg/s for 2 weeks (60,000 gallons)
/
noskip

: == transport conditions =====================================================
TRANSPORT_CONDITION Inlet
TYPE dirichlet
CONSTRAINT_LIST
0.d0 Inlet
/
/

TRANSPORT_CONDITION Initial
TYPE zero_gradient
CONSTRAINT_LIST
0.d0 Initial
/
/

TRANSPORT_CONDITION source
TYPE dirichlet
CONSTRAINT_LIST
0.d0 well
/
/
```

```
: == transport constraints ====================================================
CONSTRAINT Initial
CONCENTRATIONS
Tracer   1.e-10            F
/
/
CONSTRAINT Inlet
CONCENTRATIONS
Tracer   5.e-1             F
/
/
CONSTRAINT well
CONCENTRATIONS
Tracer 1.d0 T
/
/

: == couplers ===================================================================
BOUNDARY_CONDITION Inlet
FLOW_CONDITION Inlet
TRANSPORT_CONDITION Inlet
REGION Top
/
BOUNDARY_CONDITION Outlet
FLOW_CONDITION Initial
TRANSPORT_CONDITION Initial
REGION Bottom
/
INITIAL_CONDITION Initial
FLOW_CONDITION Initial
TRANSPORT_CONDITION Initial
REGION all
/
:skip
SOURCE_SINK Source
FLOW_CONDITION source
TRANSPORT_CONDITION source
REGION Leak
/
:noskip

: == stratigraphy ===============================================================
STRATA
MATERIAL BF
REGION BF
/
STRATA
MATERIAL HF
REGION HF
/
STRATA
MATERIAL PP
REGION PP
/
STRATA
MATERIAL URG
REGION URG
/
STRATA
MATERIAL MRG
REGION MRG
/
```

Source/sink file `src.dat`:

```
:time rate [kg/s]
0.d0      0.187e-4
1.21292e6 0.187e-4
1.21293e6 0.
1.e12     0.
```