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Title: Comparison of the Amanzi Model against Analytical Solutions and the FEHM Model

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Comparison of the Amanzi Model against Analytical Solutions and the FEHM Model

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This file documents Amanzi code verification of flow simulations for three selected cases: (1) an infinite strip aquifer embedded between two other aquifers, (2) a heterogeneous cylinder (or disc in 2D case) embedded in a background aquifer, and (3) uniform aquifers in bounded domains with fixed heads at the upper- and down-stream directions and no-flow at lateral boundaries.

The original FORTRAN codes that solve the analytical solutions for cases (1) and (2) were obtained from Greg Ruskauf. Two modifications were made for compilation on Linux systems: (a) The keyword 'mode' in OPEN statements was removed because it is not standard, and (b) variables in COMMON blocks were re-arranged to eliminate a warning message (padding of additional 4 bytes). These codes were compiled using the *gfortran* compiler on the Linux environment. Note that these analytical solutions were derived for two-dimensional problems only, and therefore in numerical simulations, we used three-dimensional domains with unit thickness for comparison.

1. Case 1: A strip of aquifer embedded between two aquifers

We consider a geological setting in which a linear infinite strip of one material is embedded between two other materials having different properties. The problem configuration is shown in plan view in Figure 1, where the domain is unbounded in both x and y directions. A pumping well is located within the infinite strip (Zone 2), and pressure responses to pumping are predicted within the domain. The analytical solution is described in Butler and Liu (1991).

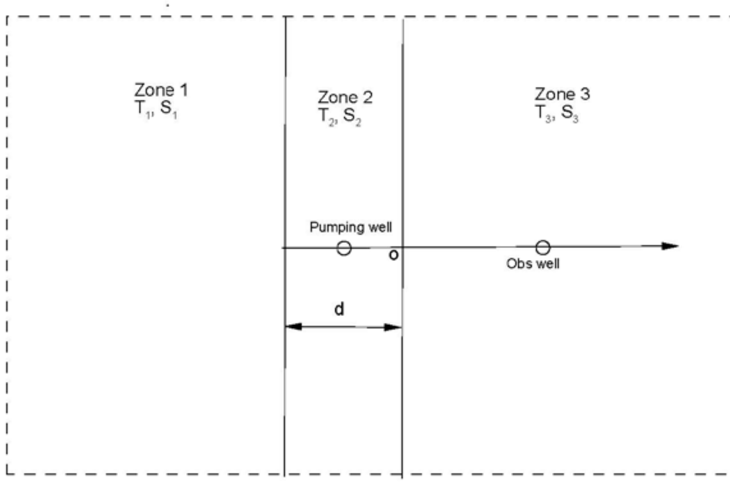

Figure 1. Configuration for a strip in an infinite domain

1.1 Comparison of analytical solution to Theis solution

The analytical solution involves the complicated numerical inversion of both a Laplace transform and a Fourier transform. Before we compare the results from this analytical solution against those from Amanzi, we first compared the accuracy of the FORTRAN code that solves the analytical solution, *strip95.f*, to the Theis solution for a special case where properties for all three materials are the same, i.e., a uniform aquifer. In this particular case, the solution should be identical to the Theis solution. Here, the y-axis lies on the boundary between material 2 and 3, and the x axis is along the line passing through the pumping well. The parameters for this case are:

> Transmissivity: T = 1000 m^2/day (=0.011574 m^2/s) for both the strip and the background materials
> Storativity: S = 2×10^{-4}
> Pumping well location (-0.5 m, 0 m)
> Pumping rate: Q = 1000 m^3/day (=0.011574 m^3/s)
> Width of the strip: d = 16 m
> Observation well location (-0.1 m, 0 m)

Here, both the pumping and observation wells are located in the strip. The comparison of dimensionless time (1/u) and dimensionless drawdown W(u) is shown in Figure 2, where $u = r^2 S / 4Tt$. The solution from the *strip95.f* code is identical to the Theis solution for 1/u > 1.0. There is some discrepancy between the two solutions when 1/u < 1.0. This is because the well function, on which the Theis solution is based,

$$W(u) = 0.577216 - \ln(u) + u - \frac{u^2}{2\cdot 2!} + \frac{u^3}{3\cdot 3!} - \frac{u^4}{4\cdot 4!} + \frac{u^5}{5\cdot 5!} - ...$$

diverges for u > 1.0 or 1/u < 1.0.

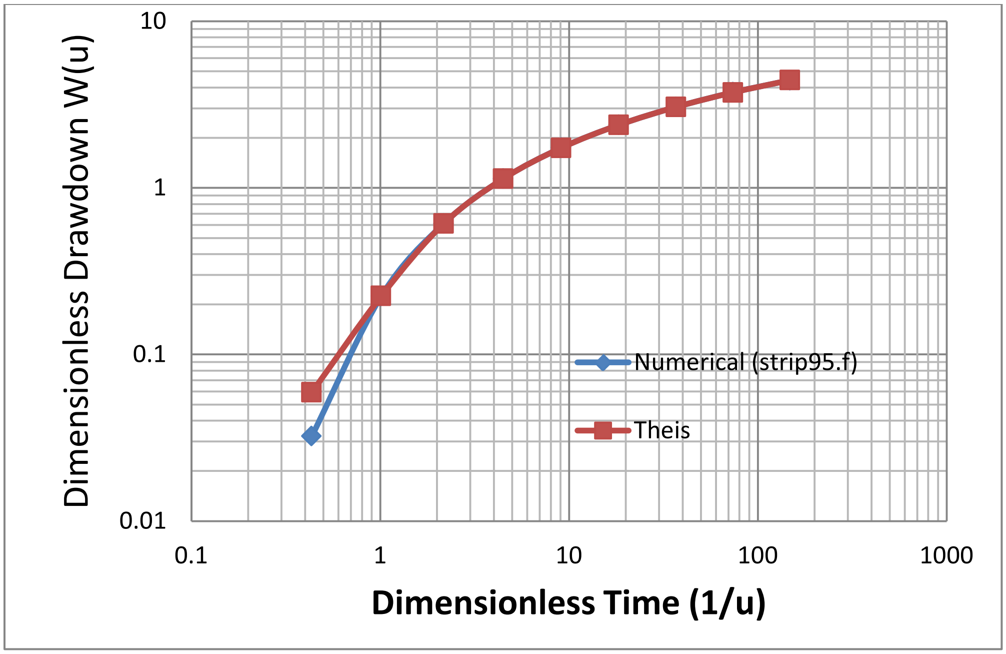

Figure 2. Comparison of the result from the strip95.f code and the Theis solution

1.2. Comparison of Amanzi to other models for uniform aquifers

Now we can compare the results from *strip95.f* with both Amanzi and FEHM for the case with uniform hydraulic properities given above. The pumping well is located at (-8 m, 0 m), and two observation wells are located at (16m, 0m) and (92m, 0m), respectively, and their corresponding distances to the pumping well are 24 m and 100 m, respectivily. Although the analytical solution is valid for infinite domains, in numerical simulators such as Amanzi and FEHM, we have to use bounded domains with fixed pressures along the boundaries for the numerical solutions. It is expected that some discrepancies between Amanzi results and analytical solutions will exist, and that such discrepancies will decrease as the domain size increases. In this study, we used two different domain sizes (defined by lower and upper corners of boxes) in Amanzi. These two corners are (-1202, -1202, 0) and (1202, 1202, 1) for domain 1, and (-1802, -1802, 0) and (1802, 1802, 1) for domain 2. The domains are discretized uniformly into 601 by 601 cells and 901 by 901 cells, which means that the grid resulution for the two domains is the same, i.e., 4 m x 4 m. An FEHM simulation using a domain size of 2400 m x 2400 m is also run for comparison. Note that there is a slight difference in the domain sizes between the Amanzi model and FEHM model because the Amanzi model is cell-based while the FEHM model is node-based. Figure 3 shows the drawdown from the analytical solution (red curves, *strip95.f*), FEHM (blue curves, 2400 m x 2400 m domain) and Amanzi (two domains) at two observation wells.

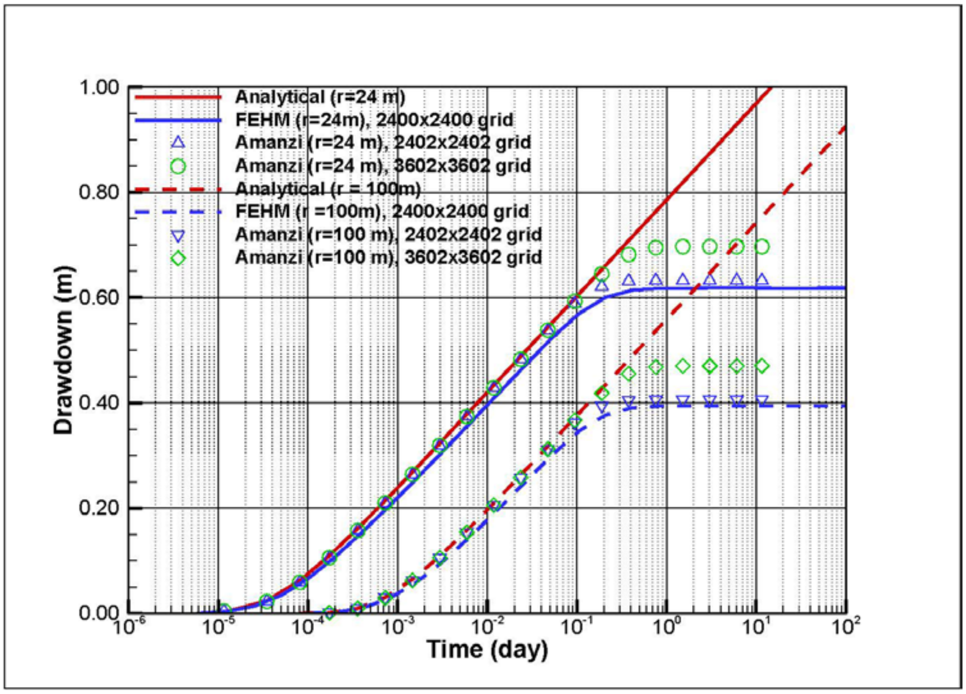

Figure 3. Comparison of drawdown calculated from the analytical solution, FEHM, and Amanzi for Case 1 with uniform hydraulic properties in the domain. Here r is the distance between the pumping well and the observation well.

It can be seen from the figure that the results from Amanzi match the analytical solution very well at earlier time. At late time, the analytical model gives an ever-increasing drawdown (because the domain is unbounded). However, in our numerical models, because of the constant head prescribed at the boundaries, the drawdown reaches steady state. As expected, the time required to reach steady state is larger for a larger domain, and the steady-state drawdown increases with the domain size. Note that the results from the Amanzi model with the same domain size match the FEHM results very well.

1.3. Heterogeneous aquifers

Next, we consider a case in which hydraulic properties vary from zone to zone:

Transmissivity: T_1 =0.11574 m^2/s; T_2 =0.011574 m^2/s; T_3 =0.0011574 m^2/s;
Storativity: $S_1 = 5\times10^{-4}$; $S_2 = 2\times10^{-4}$; $S_3 = 2\times10^{-5}$;
Pumping rate: Q = 1000 m^3/day (= 0.011574 m^3/s)
Width of the strip: d = 18 m
Pumping well location (−9 m, 0 m)
Observation well locations (15 m, 0 m) and (91 m, 0 m).

It is noted that the drawdown is very sensitive to the width of the strip. In the analytical solution the width of the strip is exact while in the numerical models the width is represented by the number of cells in the Amanzi model or nodes in the FEHM model.

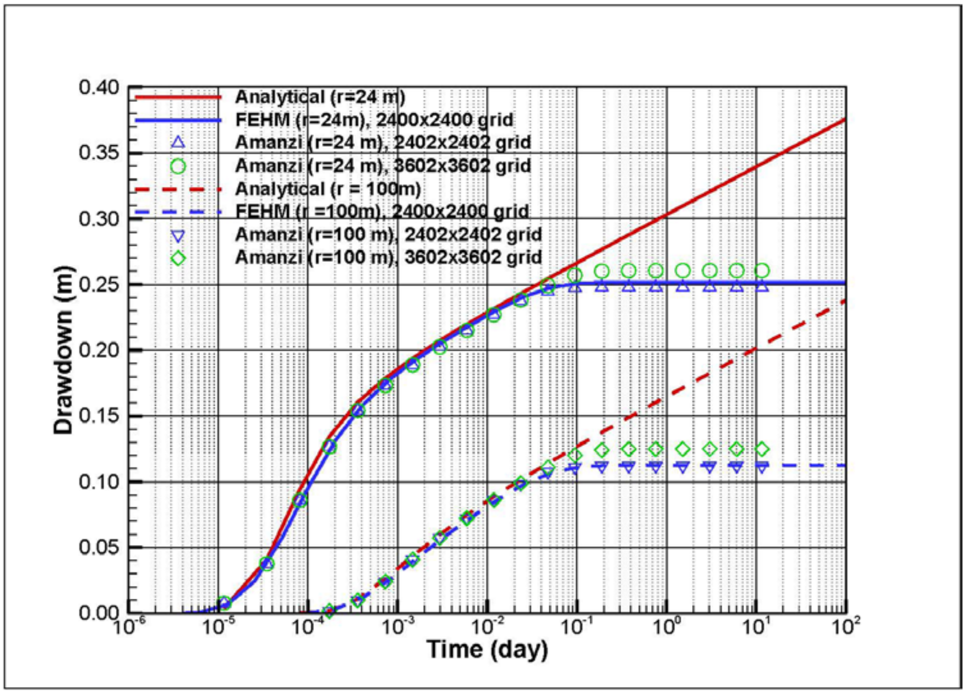

Figure 4. Comparison of drawdown calculated from the analytical solution, FEHM, and Amanzi for Case 1 with non-uniform hydraulic properties in the domain.

The comparison of the drawdown simulated by Amanzi and FEHM models and calculated from the analytical solution and simulated is depicted in Figure 4. The figure shows that the Amanzi solutions match the FEHM results very well for the same domain size.

2. Case 2: A disc of aquifer embedded into another aquifer with different hydraulic properties

We consider a geological setting in which a disc of one material is embedded in another material of different properties, as shown in Figure 5. A pumping well is located outside the disc, and pressure responses are calculated for observation wells. The analytical solution is described in Butler and Liu (1993).

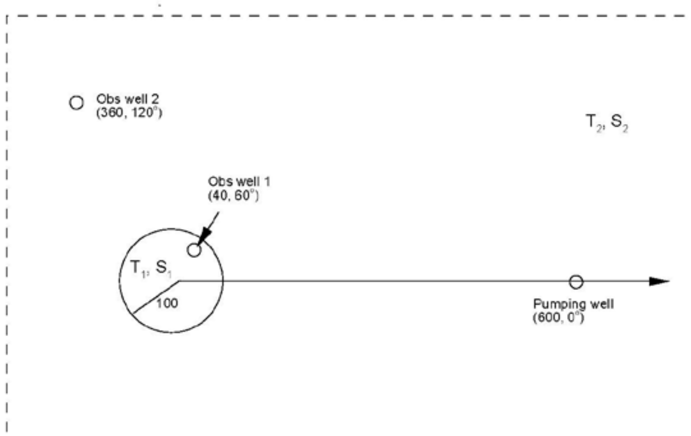

Figure 5. Problem configuration for Case 2

2.1 Uniform porous media

We first tested a special case where properties for the two materials are the same, i.e., a uniform aquifer. In this particular case, the solution should be identical to the Theis solution. The problem configuration is similar to the case in Butler and Liu (1993) with a disc radius of 100 m. The parameters for this case

Transmissivity: $T_1 = T_2 = 1000\ m^2/day$ ($=0.011574\ m^2/s$)
Storativity: $S_1 = S_2 = 2 \times 10^{-4}$
Pumping rate: $Q = 1000\ m^3/day$ ($=0.011574\ m^3/s$)
Radius of the disc: a = 100 m
Pumping well location (600 m, 0^o) in the polar coordinator with its origin at the center of the disc
Observation well 1 located at (40 m, 60^o)
Observation well 2 located at (360 m, 120^o)

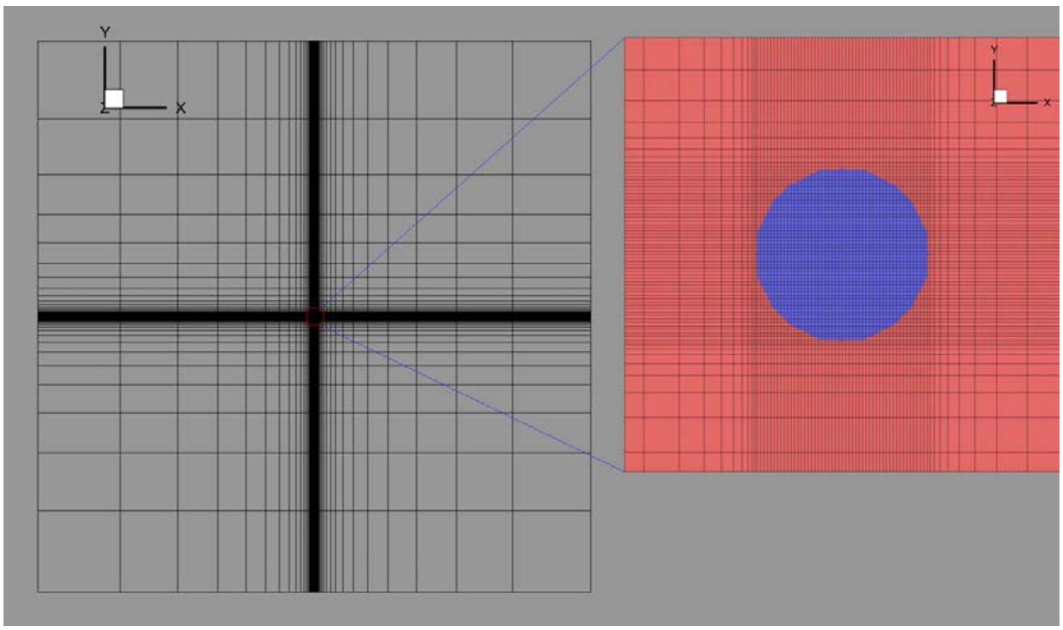

Figure 6. Numerical mesh used for both the Amanzi model and FEHM model

In numerical simulations, a non-uniform mesh was used to better present the disc (Fig. 6). To reduce the possible boundary effect, the domain size was chosen to be 20200 m x 20200 m with increasing grid spacing towards the model boundaries. The disc has a radius of 100 m, centered at (10100 m, 10100 m). The pumping well is located at (10700 m, 10100 m), and the two observation wells are at (10119 m, 10135 m) and (9921 m, 10412 m). The configuration in numerical models is compatible to that in the analytical solution.

The comparison of dimensionless time and dimensionless drawdown is shown in Figure 7. Note that, when the dimensionless time is scaled by the square of distance between the observation well and the pumping well, the dimensionless drawdown is independent of the location of the observation well, and therefore two drawdown curves for the two observation wells overlap each other.

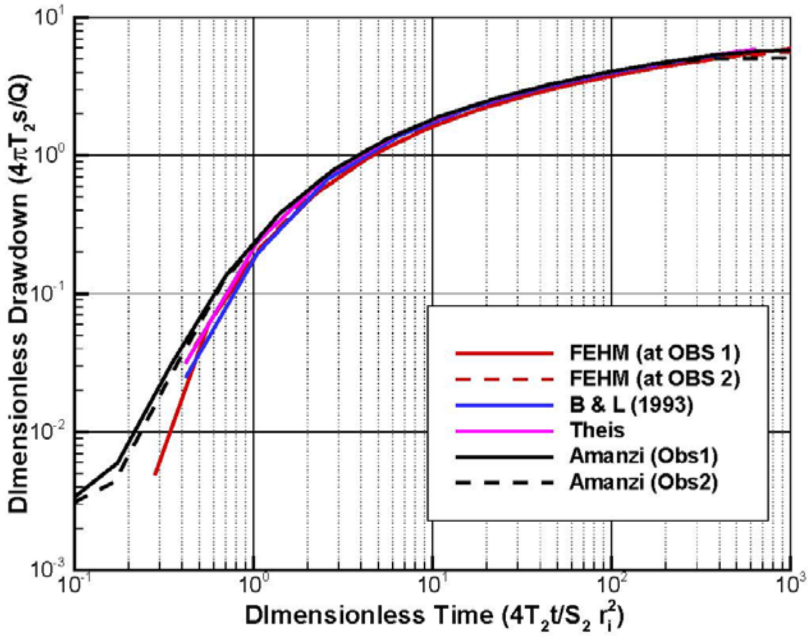

Figure 7. Good match between Amanzi results and those from analytical solutions and FEHM for Case 2 and uniform media.

2.2 Heterogeneous porous media

In the next example, all parameter values are the same as in the previous case, except that the transmissivity of the disc, $T_{1,}$ was reduced to 100 m^2/day (=0.0011574 m^2/s), which is one-tenth of T_2. Note that in this case, the Theis solution is no longer valid. We compare Amanzi results against those from the analytical solutions of Butler and Liu (1993) and from FEHM simulations. The comparison is depicted in Figure 8. Note that the dimensionless time is scaled by the square of the disc radius, and therefore the curves of dimensionless drawdown for two observation wells are different. The figure indicates that the results from the Amanzi simulations match the analytical solution very well (even better than FEHM does).

In addition, it is noted that in the code *analpod.f*, which solve the analytical solutions, the default unit for time is 'day' and the units for all other quantities should be consistent. If we use standard units in the input data, such as m^2/s for transmissivity, m^3/s for the pumping rate, and meter for length, then the corresponding time unit should be 'second'. As the result, the time scale in the output file *drdn.res* should be 'seconds', rather than 'days' as it says in the file.

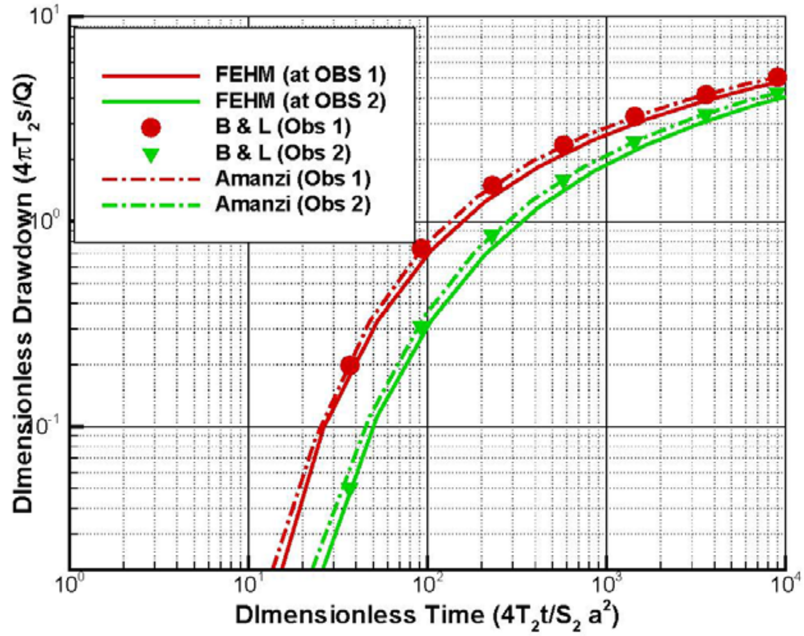

Figure 8. Good match between the Amanzi results and those from analytical solutions and FEHM for Case 2 with heterogeneous media.

3. Uniform aquifer in a bounded domain

We consider a case of pumping in a uniform aquifer with a bounded two-dimensional rectangular domain of 2400 m x 2400 m. The problem configuration is shown in Figure 9. Constant heads are prescribed on the left and right boundaries, and the no-flow condition on the lateral boundaries. Initially the head is uniform in the entire domain.

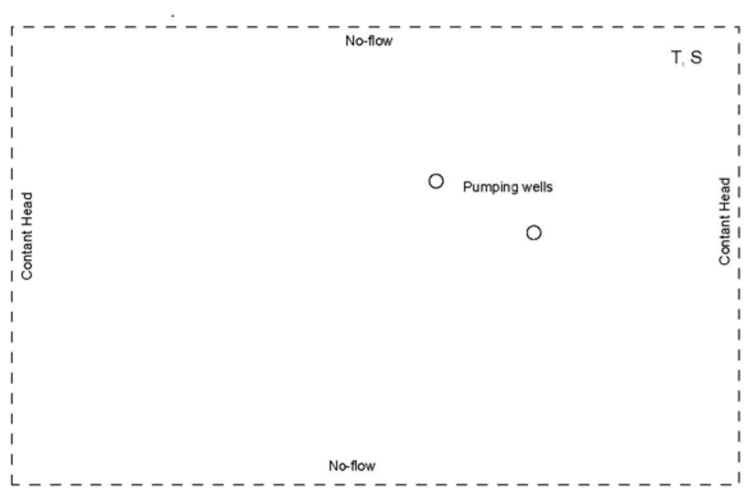

Figure 9. Problem configuration for Case 3

The analytical solution of drawdown can be written as (Lu, unpublished):

$$s = -\frac{4}{DT}\sum_{n=0}^{\infty}\sum_{m=1}^{\infty} a_n \sin(\alpha_m x)\cos(\beta_n y)\sum_{i=1}^{N_w}\frac{Q_i \sin(\alpha_m x_i)\cos(\beta_n y_i)}{\alpha_m^2+\beta_n^2} H(t-t_i)\left(1-e^{-\frac{T}{S}\left(\alpha_m^2+\beta_n^2\right)(t-t_i)}\right)$$

where α_m = mπ/L$_1$, m = 1,2,…; β_n = nπ/L$_2$, n = 0,1,2,…, $D = L_1 * L_2$, $a_0 = 0.5$ and $a_n = 1$ for $n \geq 1$, L_1 and L_2 are the domain size in x and y directions, T is the transmissivity, S is the storativity, Q_i is the pumping rate at the i-th well, t_i is the pumping starting time for the i-th well, and H(t) is the Heaviside function with H(t) = 1 for t > 0 and H(t) = 0 otherwise.

The numerical solutions from FEHM and Amanzi are compared against the analytical solution for Case 3 at two observation wells (solid lines and solid cycles for r = 24m, dashed lines and hollow cycles for r = 100 m) in Figure 10. Again, we notice that the Amanzi results match those from both the analytical solution and the FEHM simulations.

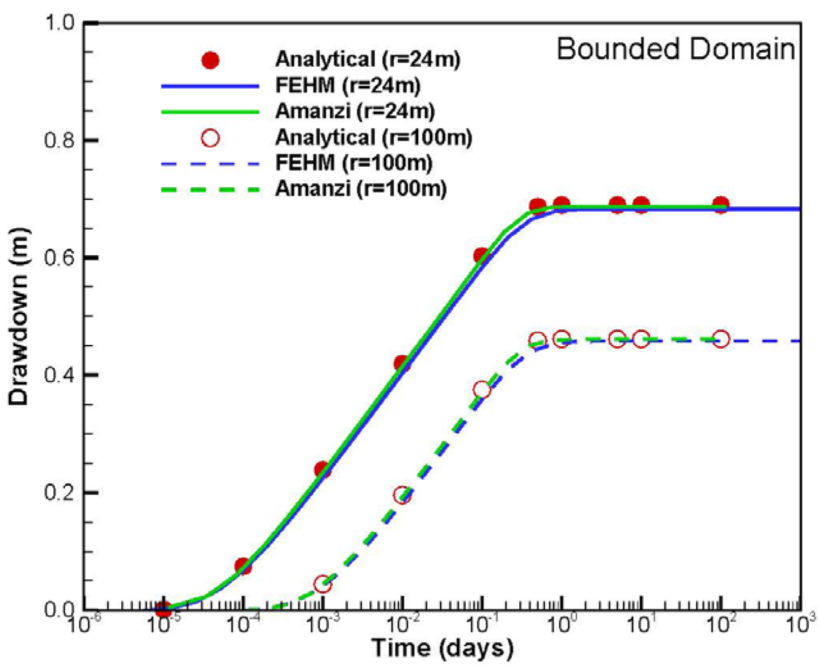

Figure 10. Comparison of drawdown at two observation wells calculated from the analytical solution and numerical simulations from Amanzi and FEHM for Case 3.

References:

1. Butler, J. J., and W. Liu, 1991. Pumping tests in non-uniform aquifers—the linear strip case, Journal of Hydrology, 128, 69-99.
2. Butler, J. J., and W. Liu, 1993. Pumping tests in nonuniform aquifers: the radially asymmetric case, Water Resources Research, 29 (2), 259-269.