Sensitivity analysis of aquifer parameter estimations based on the Laplace equation with linearized boundary conditions

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[1] Estimates of aquifer parameters, saturated hydraulic conductivity, and drainable porosity were obtained by an analytical solution of the two-dimensional Laplace equation with linearized boundary conditions and were compared to prescribed parameters in a finite element model that simulated drainage of a coupled system of unsaturated/saturated flow. Boundary conditions prerequisite for the analytical solution were systematically relaxed during numerical experiments to see how the resulting aquifer-parameter estimates deteriorate if (1) correct aquifer geometry values are used and (2) aquifer geometry is imprecisely estimated. Sensitivity of aquifer parameter estimation to imprecise saturated thickness and groundwater profile information was also performed at the watershed scale. The analysis supports the robustness of the saturated hydraulic conductivity and drainable porosity estimates in all cases considered, at both field and catchment scales, with the only exception being the drainable porosity for sand where a significant flux-exchange between the vadose and phreatic zones during drawdown results in both modeled and estimated effective drainable porosities significantly larger than traditionally expected. *INDEX TERMS:* 1829 Hydrology: Groundwater hydrology; *KEYWORDS:* Laplace equation, aquifer parameter estimation, sensitivity analysis

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1. Introduction

[2] In an ideal world of modeling, one obtains information on the characteristics of the processes to be modeled at the same scale as the problem occurs. This, however, becomes the exception in hydrology with increasing scale of the problem. In many occasions information on aquifer characteristics is only available at a scale several magnitudes smaller than the scale of the problem at hand. It is not rare that entire aquifer systems, such as the High Plains aquifer in the United States, with a characteristic length of 10^5 m are modeled numerically using saturated hydraulic conductivity and/or porosity values from grain size analysis, slug, bail or pumping test results [*Gutentag et al.*, 1984].

[3] Existing techniques [*Glover*, 1960; *Brutsaert and Nieber*, 1977; *Brutsaert and Lopez*, 1998; *van de Giesen et al.*, 1994; *Parlange et al.*, 2001] that estimate, e.g., the saturated hydraulic conductivity at the field or watershed scale have largely been overlooked in the past in favor of pumping test analyses. The reason for this neglect may be at least threefold. First, the estimates that these techniques provide are generally one-to-two magnitudes larger than those of grain size or pumping test results [*Troch et al.*, 1993]. The discrepancy lately is attributed to the recently much-discussed presence of preferential flow and flow in macropores [*Troch et al.*, 1993; *Brutsaert and Lopez*, 1998] in the field or watershed. The effects of these may be incorporated in the field/catchment-scale estimates but not necessarily in the pumping test results. Second, most field/catchment-scale estimation techniques involve the Boussinesq equation, which is a nonlinear partial differential equation by nature, and so analytical solutions exist only in special cases, which may automatically be associated with ''limited practical interest'' [*Strack*, 1989]. Third, field/catchment-scale estimates are hard to verify, unlike slug, bail, or pumping test results, for which material samples can be collected and tested in the laboratory. However, one way field-to-catchment-scale parameter estimates could be verified is by using them in existing hydrologic/hydrogeologic models to see if they result in better behavior of the modeled phenomena as opposed to aquifer parameter estimates obtained at a smaller scale. Another possibility, which will be pursued here, is to apply the parameter estimation technique to numerical simulation results and check how it predicts the original parameters that were prescribed in the model [*Szilagyi et al.*, 1998]. This way the numerical model not only generates groundwater discharge values, but its aquifer parameters serve as ''ground truth observations'' against which parameter estimation results of existing analytical techniques can be verified.

[4] In the following, the parameter estimation capability of the analytical solution [*van de Giesen et al.*, 1994] of an aquifer drainage problem will be tested. Of particular interest is how the estimates deteriorate with relaxation of some of the boundary conditions prerequisite to the solution and also, with incorrect estimation of necessary geometrical and hydrological properties of the aquifer. By doing this, the applicability of the technique may become more general provided the estimates are robust, meaning that they are not very sensitive to specific boundary conditions and to errors

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in additional parameter values required for the analytical solution.

[5] The governing equation of flow in a saturated porous medium is the Laplace equation [*van de Giesen et al.*, 1994], which is now written for a two-dimensional case

$$\frac{\partial^2 H(x,y,t)}{\partial x^2} + \frac{\partial^2 H(x,y,t)}{\partial y^2} = 0 \qquad (1)$$

where H is the total hydraulic head, x and y are the horizontal and vertical coordinates and t is time. Equation (1) is subjected to the following initial and boundary conditions:

$$\begin{gathered} H(x,y,0) = h_B; \quad H(0,y,t) = h_0, t > 0 \\ \partial H(x,0,t)/\partial y = 0; \quad \partial H(B,y,t)/\partial x = 0 \\ H(x,y,t) = y = h(x,t) \quad \text{at the free surface} \end{gathered} \qquad (2a)$$

where B is aquifer width, h_B is the initial flat equilibrium water level in the ditch (or stream) and in the aquifer, h_0 is the value to which the initial water level in the ditch drops (supposedly) instantaneously (Figure 1), and h is elevation of the groundwater, a function of distance from the ditch and of time. All elevations are relative to the underlying horizontal impermeable layer. If the changes in h in the x-direction are small compared to the characteristic depth ($\approx h_0$), of the saturated zone, then the boundary condition on the phreatic surface is given by the following linear partial differential equation [*van de Giesen et al.*, 1994]

$$f\frac{\partial h}{\partial t} = -k_{\text{sat}}\frac{\partial H}{\partial y} \qquad (2b)$$

where f is the drainable porosity or specific yield of the aquifer, and k_{sat} is the saturated hydraulic conductivity, both assumed to be scalar constants in time. It is further assumed here that there is no contribution to the flow from the vadose zone [*van de Giesen*, 1994].

[6] The aquifer discharge, Q, to the ditch in the problem defined by (1)–(2b) is given as [*Van de Giesen et al.*, 1994]

$$Q(t) = \sum_{n=1,3,\ldots}^{\infty} k_{\text{sat}}\frac{4(h_B - h_0)}{n\pi}\tanh\left(\frac{n\pi h_0}{B}\right) \cdot \exp\left(-\frac{k_{\text{sat}}}{f}\tanh\left(\frac{n\pi h_0}{B}\right)\frac{n\pi}{B}t\right) \qquad (3)$$

which contains five parameters: k_{sat}, f, B, h_0, and $\Delta h = h_B - h_0$. Note that (3) describes aquifer drainage for a fully penetrating ditch/stream case. One can obtain estimates of k_{sat} and f by fitting (3) to measured ditch or stream discharge data through systematically trying different combinations of the k_{sat} and f values in search of a best fit, provided one has estimates of the aquifer width, B, the average saturated thickness ($\approx h_0$) of the aquifer and Δh. When (3) is applied in a field-setting, B is one-half of the width of the field drained by ditches at the two sides. When (3) is applied to obtain catchment-scale estimates of f and k_{sat}, then the aquifer width can be calculated [*Brutsaert and Nieber*, 1977; *Troch et al.*, 1993; *Szilagyi et al.*, 1998] as $B = (2\,R_d\,)^{-1}$, where R_d is the drainage density defined [*Horton*, 1945] as $R_d = LA^{-1}$, where L is the total length of the contributing streams, and A is the contributing watershed area. *Szilagyi et al.* [1998] showed with the help of numerical simulations that such estimation of B in a watershed setting did not affect the robustness of the aquifer parameter estimates obtained by approximate analytical solutions of the Boussinesq equation [*Brutsaert and Nieber*, 1977].

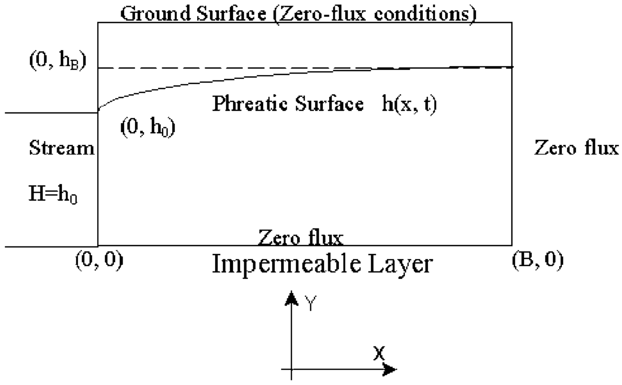

Figure 1. Schematic of the stream-aquifer system with full stream penetration and the boundary conditions applied in the numerical simulations.

[7] When the ditch (or stream) that drains the aquifer is fully penetrating, h_0 in (3) is the mean or characteristic water depth of the ditch/stream during drainage or during drought flow for streams. However, partial aquifer penetration is a much more common condition than full penetration and so it becomes a question whether (3) may still give acceptable aquifer parameter estimates in this more general case, and if so, how close the estimates will be to their true values and what geometric properties the parameters will be the most sensitive to. Note that in this general case, h_0 is the mean saturated thickness under the ditch/stream, plus the mean ditch- or stream water depth during recession flow. The saturated thickness and full or partial penetration condition of the ditch/stream may not always be known; thus one may resort to estimating h_0 by the mean water depth in the ditch/stream during aquifer drawdown. Estimating the saturated thickness in (3) this way may not be that critical after all, since (3) has the h_0 term as the argument of the hyperbolic-tangent function, which goes to unity rather quickly with increasing n values in the summation. When no information on the saturated thickness is available, the other term, $h_B - h_0$ in (3) must also be estimated in practical applications, where h_B can be taken as the mean elevation (above the ditch/stream bottom) of the water divide between the streams reduced by the mean thickness of the vadose zone. The sensitivity of aquifer property estimates to imperfect boundary conditions and/or imprecise saturated thickness data can only be evaluated, in lieu of measurable field-scale values of k_{sat} and f, if one compares the estimates given by (3) to prescribed parameters of a numerical model that simulates aquifer drainage under a partial-penetration condition.

2. Methodology

[8] Two-dimensional aquifer drainage was simulated by a finite element model that numerically integrated the

Table 1. Parameter Values in the Campbell Model[a]

Soil Texture	φ	k_{sat}, cm/s	k_{sat}, m/d	$\lvert\psi_{ae}\rvert$, cm	$\lvert\psi_{ae}\rvert$, kPa	b
Sand	0.395	1.76×10^{-2}	15.21	12.1	1.18	4.05
Loam	0.451	6.95×10^{-4}	0.60	47.8	4.68	5.39
Clay	0.482	1.28×10^{-4}	0.11	40.5	3.97	11.4

[a]After *Clapp and Hornberger* [1978].

combined unsaturated/saturated flow equation [*Lam et al.*, 1987]

$$\frac{\partial}{\partial x}\left(k(\psi)\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(k(\psi)\frac{\partial H}{\partial y}\right)=m\gamma\frac{\partial H}{\partial t} \tag{4}$$

where k, a function of ψ, the suction/pressure head, here may denote both unsaturated and saturated hydraulic conductivities; m is the slope of the water retention curve (volumetric water content, θ, versus suction) at a given ψ value, which becomes the coefficient of volume change in the saturated zone [*Lam et al.*, 1987]; γ is the unit weight of water; and H as before is the total hydraulic head. In the numerical integration of (4), it was assumed that pore-air pressure remains atmospheric at all times.

[9] The drainage simulations at the field scale were accomplished with a 1-m thick vadose zone of three different physical soil texture types: sand, loam, and clay. The water retention, $\psi - \theta$, and the $k - \theta$ curves for the different texture types were estimated using the power law equations of *Campbell* [1974] for simplicity

$$|\psi(\theta)| = |\psi_{\alpha\varepsilon}|\left(\frac{\varphi}{\theta}\right)^b \tag{5a}$$

$$k(\theta) = k_{\text{sat}}\left(\frac{\theta}{\varphi}\right)^c \tag{5b}$$

where ψ_{ae} is the air entry suction, φ is the total porosity, b is the often-called pore size distribution index, c ($\approx 2b + 3$) is the so-called pore-disconnectedness index, and k_{sat} is the assumed saturated hydraulic conductivity of the given soil and the underlying phreatic zone. The values of the parameters for the three types of soil texture used in the numerical model are listed in Table 1. Figure 2 displays the resulting $\psi - \theta$, and $k - \theta$ curves. The hydraulic property curves were extended for suctions smaller than the air-entry value by near-constant segments. The numerical model extends the $\psi - \theta$ curve into the saturated zone by a linear extrapolation of θ, while prohibiting vanishing slopes [*Lam et al.*, 1987]. The three physical soil textures (sand, loam, and clay), through their defined physical properties, correspond to the following aquifer material types: clean sand, silty sand, and silt [*Freeze and Cherry*, 1979; *Fetter*, 2001] in the saturated zone.

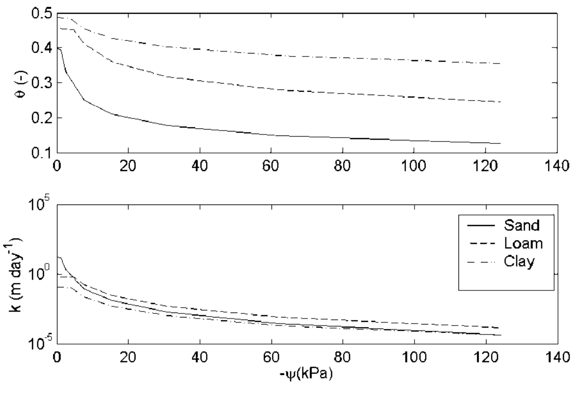

Figure 2. Hydraulic properties of the physical soil textures of the vadose zone used in the numerical model.

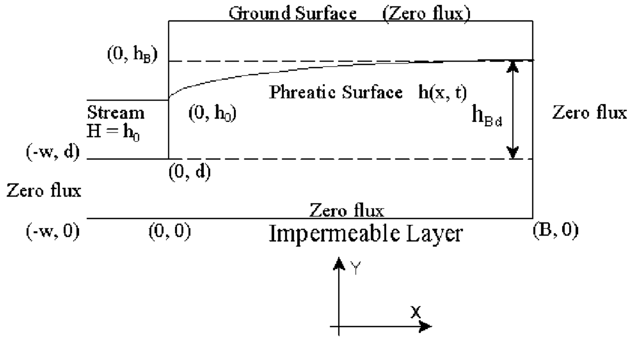

Figure 3. Schematic of the stream-aquifer system with partial stream penetration and the boundary conditions applied in the numerical simulations.

[10] To check how (3) predicts aquifer properties under more general conditions that is required by the analytical solution, full penetration of the ditch draining the aquifer was abandoned. This change brought with it two extra parameters that may influence the drainage: the half-width of the ditch, w, and the distance of ditch-bottom from the impervious layer, d (Figure 3). Also of interest was if the initial saturated thickness, h_{Bd}, above the ditch-bottom interacted with these two new parameters in the estimated aquifer properties, k_{sat} and f. For w, four values were considered: 0.1, 0.5, 1, and 3 m; while for d the following four values were chosen: 0.1, 1, 5, and 10 m. This meant $4 \times 4 = 16$ unique combinations. The combinations were repeated for the following four h_{Bd} values: 3, 5, 7, and 9 m, which for the three different soil types (and the corresponding aquifer material types) meant altogether $16 \times 4 \times 3 = 192$ unique combinations for each of the two scenarios considered. In the first scenario, h_B and h_0 were assumed to be known, and were calculated as $h_B = d + h_{Bd}$, and $h_0 = d + h_{Bd} - \Delta h$, respectively. In the second scenario, h_0 was taken equal to the ditch-water depth, i.e., $h_0 = h_{Bd} - \Delta h$, in the curve-fitting procedure, thus simulating a case when the ditch is incorrectly assumed to be fully penetrating.

[11] Each numerical simulation out of the 384 total started with a flat groundwater profile with $\Delta h = 0.2$ m, and an aquifer width of $B = 20$ m. Note that the chosen values of Δh, h_0, h_B and B ensure that the linearization of the free boundary introduces only a small error into the analytical calculations, since $\Delta h \ll h_0$, $h_0/h_B > 0.7$ and $B/h_B > 1$, as required [*van de Giesen et al.*, 1994; *Polubarinova-Kochina*, 1962]. The aquifer discharge, Q, was calculated by two different methods to make sure that the numerical results were correct: (1) by a water balance

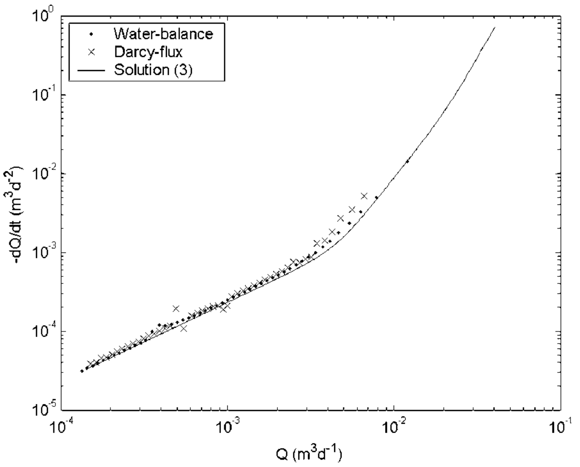

Figure 4. The Q versus $-dQ/dt$ values of a clay/silt aquifer of unit length during drainage. Solution (3) is with the k_{sat} and f values of Tables 1 and 2. The outflow values, Q, were calculated by (1) using a water balance of the coupled unsaturated/saturated system and (2) integrating Darcy-fluxes along the stream/aquifer and atmosphere/aquifer interfaces. Here Δh = 0.1 m, B = 6 m, h_B = 1 m, and the vadose zone is 1 m thick.

approach, where the discharged water volumes between two consecutive time increments were taken equal to the change in the total water content of the coupled unsaturated/saturated system in the time interval, and; (2) by integration of the Darcy fluxes along the total stream-aquifer interface and the aquifer-atmosphere interface (which also includes the seepage face) from stream level up to the ground surface.

[12] The effect of imprecise information of the saturated thickness, h_0, on aquifer parameter reliability was also investigated at the watershed scale. The scale distinction between field and catchment scales is necessary only because the speed at which the argument of the hyperbolic-tangent function goes to unity is influenced by the h_0/B ratio; thus sensitivity of aquifer parameter estimates to imprecise h_0 information may be scale-dependent. At the catchment scale, Dupuit's assumption of constant hydraulic heads along verticals is often invoked, in which case the groundwater flow is considered mainly horizontal. Since (3) predicts aquifer drainage under different saturated thickness conditions, it can readily be checked by using these values as "observations," how aquifer parameter estimates are influenced if incorrect h_0 values are used in the estimation procedure of fitting (3) over the "observations." Note that in this case the question of full or partial penetration does not enter the problem, because under Dupuit's condition they are considered the same. Three different B values were used in the analysis: 200, 400, and 800 m. The middle value of 400 m is the average characteristic distance from stream to divide over 22 catchments in the U.S. Department of Agriculture-Agricultural Research Service (USDA-ARS) Washita Experimental Watershed complex in the Chickasha region of central Oklahoma [*Brutsaert and Lopez*, 1998] where the watersheds range in size from 1.02 km^2 to 538.19 km^2.

[13] The following h_0 values were used in the sensitivity analysis: 0.5, 1, 5, and 10 m, while during curve fitting an

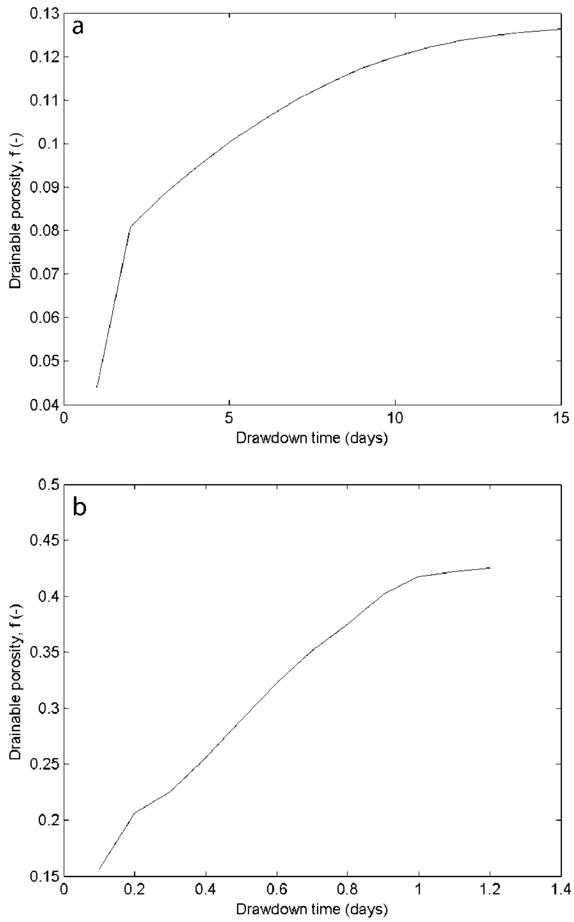

Figure 5. (a) Changes in modeled drainable porosity during drainage of a clay/silt aquifer with an initial vadose zone thickness of 3 m, h_B = 1 m, Δh = 0.1 m, and B = 6 m. (b) Changes in modeled drainable porosity during drainage of a sand aquifer with an initial vadose zone thickness of 1.7 m, h_B = 1 m, Δh = 0.1 m, and B = 6 m.

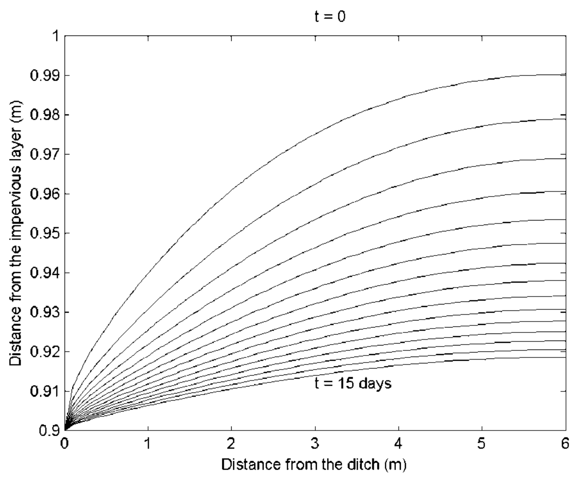

Figure 6. Changes in groundwater profile through time for the aquifer in Figure 5a with dt = 1 d.

Table 2. Drainable Porosity Values, $f = \theta(\psi = 0 \text{ kPa}) - \theta(\psi = -124 \text{ kPa})$, as a Function of Soil Texture

Soil texture	f (-)
Clay	0.131
Loam	0.21
Sand	0.274

h_0^{est} value of 0.5 m was used in all (3 × 4 = 12) cases. The Δh values in (3) were chosen as $B/100$, satisfying the general practical requirement of groundwater slope of 1:100 for Dupuit's condition [*Verruijt*, 1982].

[14] The last parameter investigated at the watershed scale in the present sensitivity analysis was the Δh term in (3). It was checked how the k_{sat} and f estimates behaved when Δh_{est} was set to 0.1, 0.5, 1, 2, 4, and 8 m in the curve-fitting procedure instead of the correct Δh = 1 m value while h_0 was set equal to 1 m.

3. Results and Discussion

[15] When trying to fit the analytical solution (3) to measured data, one faces the difficulty of not knowing the starting time of real aquifer drainage due to delays between the cessation of precipitation and the build-up of groundwater storage. *Brutsaert and Nieber* [1977] thus recommended the elimination of time in the drainage analysis by plotting aquifer discharge, Q, against the change of discharge rates, dQ/dt. If the resulting value-pairs of (3) are plotted on a double-logarithmic graph, then the initially large slope in early times of the drawdown will transform rather rapidly into a slope of unity as time progresses (Figure 4). Note that for the slope-change to occur and thus the practical fitting of the analytical curve to the measured values be possible, no initial horizontal water level (and a sudden drop in the ditch/stream level) is necessary. The slope change develops when the receding groundwater profile reaches the water divide, consequently a near horizontal water table around the water divide ensures the necessary change in the slope.

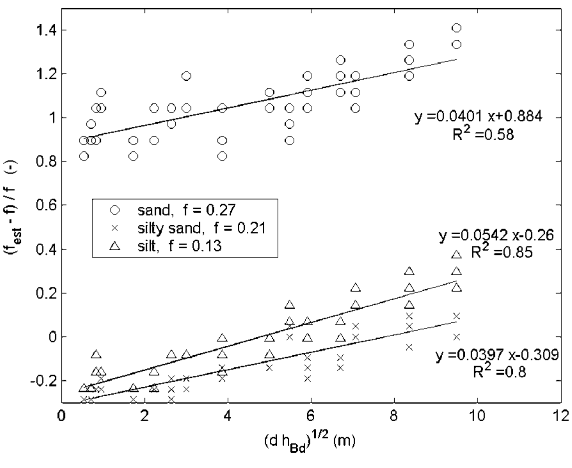

Figure 8. Sensitivity of the drainable porosity estimates to aquifer geometry under partial stream penetration.

[16] In each simulation out of the 384 cases, the analytical solution (3) was fitted to the numerical model values in a mean squared-error sense to obtain estimated values of k_{sat} and f. Because the water balance-derived values (dots) generally displayed less scatter (Figure 4), solution (3) was always fitted to these values in each case considered. The "quasi-instantaneous" drainable porosity value, defined as drained water volume over volume change in the saturated zone [*Fetter*, 2001] in a given, arbitrarily short time period, is influenced by the flux-exchange between the vadose and phreatic zones [*Freeze and Cherry*, 1979] (Figure 5a). As the groundwater table (marked by ψ = 0) changes its position ever slower when approaching its final flat position due to drainage (Figure 6), the relative importance of the unsaturated-flow contribution to the phreatic zone and so to drainage may become more apparent, resulting in a "quasi-instantaneous" drainable porosity value of the coupled system at those times surpassing the constant total porosity value (φ = 0.395, see Table 1) of the aquifer, defined by the water retention curve (Figure 2 and Table 2).

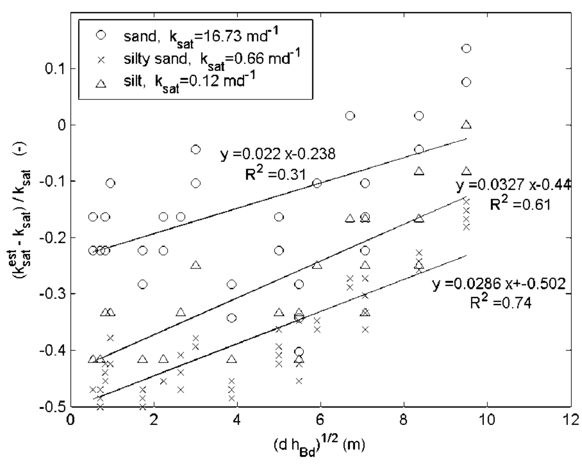

Figure 7. Sensitivity of the saturated hydraulic conductivity estimates to aquifer geometry under partial stream penetration.

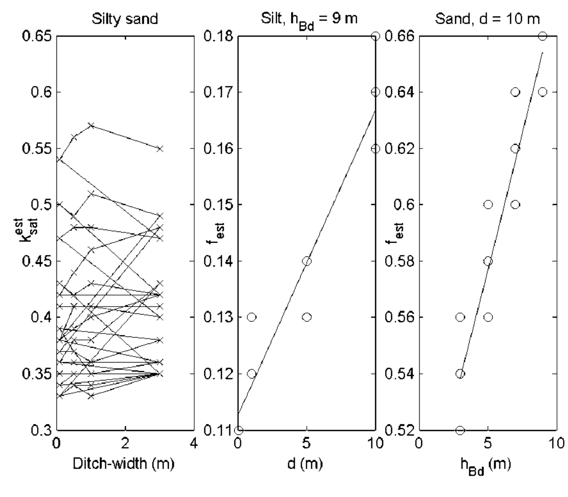

Figure 9. Partial results of the sensitivity analysis of the aquifer parameters to individual aquifer geometry characteristics.

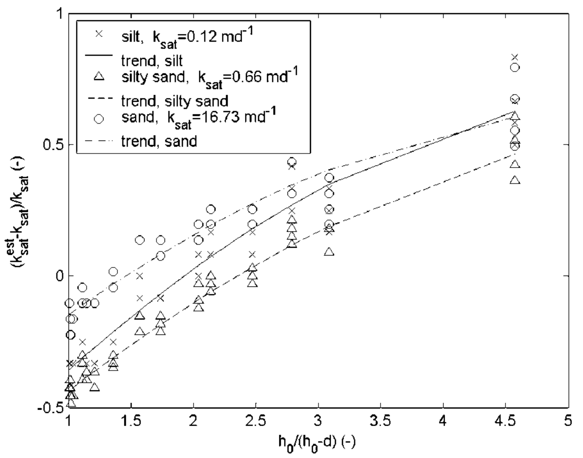

Figure 10. Sensitivity of the saturated hydraulic conductivity estimates to incorrect saturated thickness (h_0) estimates under partial stream penetration. The lines are the best fitting second-order polynomial curves.

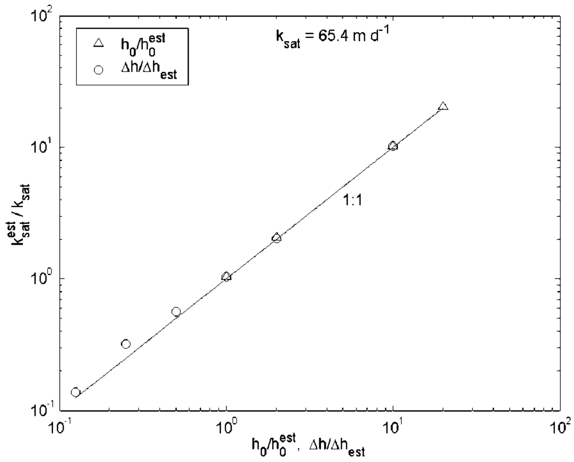

Figure 12. Sensitivity of the saturated hydraulic conductivity estimates to incorrect initial estimation of the saturated thickness (h_0) and Δh at the watershed scale; h_0^{est} = 0.5 m, Δh = 1 m.

[17] Figures 7 and 8 display the relative error in the saturated hydraulic conductivity and drainable porosity estimates at the field scale when correct aquifer geometry and saturated thickness values were used in (3) during curve fitting. The estimates are about evenly and only slightly sensitive to the two aquifer geometry parameters, d and h_{Bd}, under partial penetration; and the relative error of the estimates is directly related to their combined values. Interestingly, stream- or ditch-width, w, does not influence the estimates (Figure 9) which are generally close to the model prescribed values, with an apparent slight bias in the saturated hydraulic conductivity estimates. The only exception is drainable porosity of the sand aquifer. Because unsaturated flow contribution to drainage is least negligible in the sand-aquifer case, (3) accounts for this extra drained water volume and compensates for it by a higher drainable porosity value during curve fitting.

[18] Figures 10 and 11 display the relative errors in the aquifer-parameter estimates as a function of the error made in the saturated thickness, h_0, estimation. The abscissa is the ratio of the actual saturated thickness over the characteristic ditch-water depth that serves as the estimate of h_0 when no information is available of the saturated thickness or of the penetration condition of the ditch. As it can be seen, the relative error of the estimations is small, even when the real saturated thickness is more than four-times larger than its assumed value in (3) during curve fitting. In the saturated hydraulic conductivity case, more than 95% of the estimated values are within the interval [$-0.5k_{sat}$; $0.5k_{sat}$]. This range is even smaller for the drainable porosity estimates: [$-0.3f$; $0.3f$], with the exception of the sand-aquifer case, most probably for reasons mentioned above.

[19] Reliability of (3) at the watershed scale was tested with a k_{sat} value of 65.4 m d^{-1}, and an f value of 0.0167, representative mean catchment-scale values for the Washita

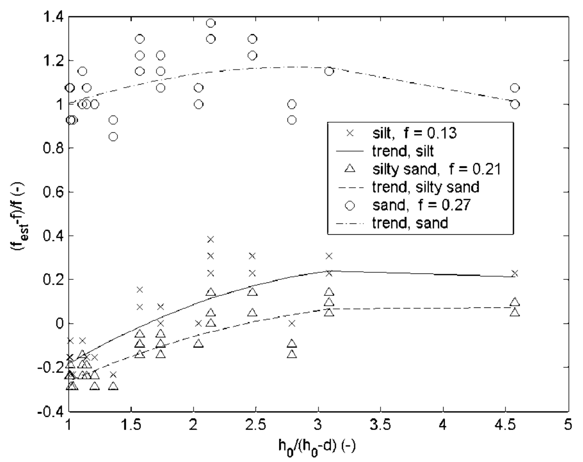

Figure 11. Sensitivity of the drainable porosity estimates to incorrect saturated thickness (h_0) estimates under partial stream penetration. The lines are the best fitting second-order polynomial curves.

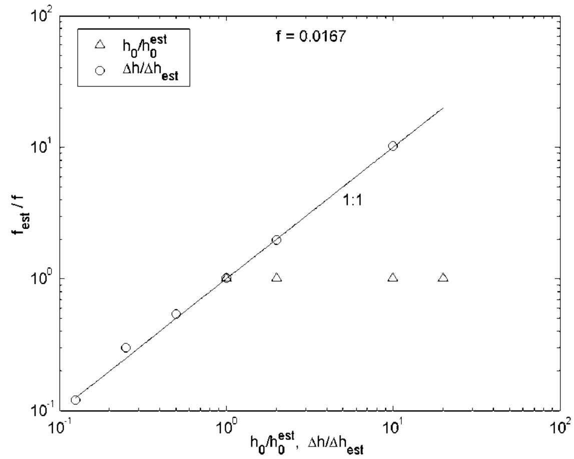

Figure 13. Sensitivity of the drainable porosity estimates to incorrect initial estimation of the saturated thickness (h_0) and Δh at the watershed scale. h_0^{est} = 0.5 m, Δh = 1 m.

Experimental Watershed complex [*Brutsaert and Lopez*, 1998]. Figures 12 and 13 display the sensitivity of the saturated hydraulic conductivity and drainable porosity estimates to incorrect (i.e., estimated) information of h_0 and Δh for B = 800 m. The other two aquifer-width cases (B = 200 and 400 m) gave identical results. As it turns out, k_{sat} is linearly related to errors made in the h_0 and Δh values, respectively. The same is true for f in relation to errors in Δh, but the drainable porosity estimates were not influenced at all by errors made in the h_0 value. A linear error propagation in the k_{sat} estimate to incorrect information of the saturated thickness is a direct consequence of the linear boundary condition in (2b). Since Δh is outside of the hyperbolic-tangent and exponential-function arguments that contain the aquifer width value, B, in (3), the results of this last case of sensitivity analysis are expected to be valid at the field scale as well.

[20] In conclusion, it can be said that the application of the analytical solution [*van de Giesen et al.*, 1994] of Laplace's equation of drainage to estimate field- and watershed-scale aquifer properties (saturated hydraulic conductivity and drainable porosity) is proved to be a robust estimation method. Verification was accomplished using a finite element numerical model that simulated drainage of the coupled systems of unsaturated/saturated flow. The constant, scalar-valued aquifer parameters prescribed in the numerical model served as ''ground truth observations'' of aquifer characteristics. The estimates were only slightly sensitive to errors made in the parameter values or boundary conditions required by the solution. In cases where the flux-exchange between the vadose and phreatic zones was not negligible, such as in sand aquifers, the parameter estimation resulted in increased values of the drainable porosity, reflecting water contribution from the vadose zone in the drainage process. It is hoped that the current technique and/or similar ones, such as by *Brutsaert and Lopez* [1998] or by *Parlange et al.* [2001], due to their favorable properties and ease of use, will complement smaller scale methods currently used for aquifer evaluation.

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