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SUBJECT: HARMONIC MEAN AND FLOW PARAMETERS FOR FDM GROUNDWATER MODELS

The recent SWIFT II training seminar offered an opportunity for presentation of some of the model's numerical techniques. One issue briefly discussed was the use of harmonic mean for "transmissibility" calculations. This memo is an attempt to continue that discussion and suggest some alternative techniques.

During finite difference solution of porous media flow equations, it is necessary to compute the interblock (for grid-centered) or interface (for block-centered) product of cross-sectional area and hydraulic conductivity. If values are specified for each block, the interface value must be computed as some average of the block values. In general, the best technique for computing these averages is that which results in head differences and fluxes closest to an analytical solution. The analytical solution for flow between two blocks depends on the properties of the system and how those properties vary <u>between</u> blocks.

One assumption for the variation of properties between blocks is that properties are constant over each block and changes occur (abruptly) only at the block interface. The effective hydraulic conductivity or effective block height (assuming other properties constant) for the block interface in this system is <u>exactly</u> equal to the harmonic mean of hydraulic conductivities or heights (see Bear, 1979 p. 81). SWIFT II (Reeves et.al., 1983) uses harmonic mean for hydraulic conductivity and block height.

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An alternative second assumption is that properties vary linearly between nodes or block centers. In this case, as shown in Attachment A, the geometric and arithmetic mean are better estimates of the effective interface value than the harmonic mean. Haverkamp and Vauclin (1979) discuss the estimation of interblock hydraulic conductivity and recommend use of geometric mean. Attachment B presents an averaging procedure which, like the harmonic mean for blocky systems, yields an exact effective interface value for linear variation between nodes. Although this technique may, in some instances, provide the most accurate results, we know of no code which uses it.

The issue of the choice of averaging technique is a current one and has not been definitively resolved. For example, Milly (Prof. Chris Milly, Princeton, personal communication, 1983) reports instability in unsaturated flow models using geometric mean. No doubt, alternative conceptualizations of property variation between blocks will yield different "best" estimators.

Given the current work in estimating interblock flow properties, and the suitability of alternative techniques for at least one realistic conceptualization, we feel that it is important to discuss incorporation of some of these alternative techniques into SWIFT, SWIFT II and other codes used by NRC.

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Attachment
As stated

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DATE	12/21/83	12/21/83					

Draft No. 1 (DM) 83/11/28

Draft No. 2 (DM) 83/11/29

References: Bear, Jacob, Hydraulics of Groundwater, McGraw-Hill, New York, 1979.

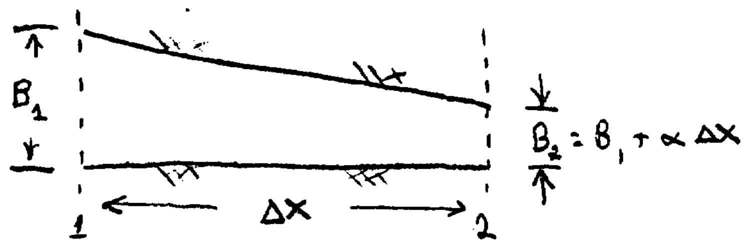
Haverkamp, R., and M. Vauclin, A note on estimating finite difference interblock hydraulic conductivity values for transient unsaturated flow problems, Water Resources Reaearch 15(1), 181-187, 1979.

Reeves, Mark, N. D. Johns, and R. M. Cranwell, Theory and implementation for SWIFT II, Release 3.83, DRAFT Sand 83- , 1983.

Attachment A

Estimates of interblock flow parameters with linear variation between nodes

Consider steady-state one-dimensional flow in a layer with changing thickness (see Figure).



Vertical flow components are ignored. For finite difference methods, layer thickness, B, is specified at the node points. Computation of flux between node "1" at $x=x_1$ and node "2" at $x=x_1 + \Delta x$ requires the estimation of effective layer thickness between 1 and 2. The goal of estimating effective layer thickness, B', is not that the actual layer thickness at the interface between 1 and 2 be computed accurately (i.e., B' = B, + $\alpha\Delta x/2$), rather it is that the computed head values and fluxes are accurate. To evaluate this accuracy, we can compute the change in head from 1 to 2 for a given flux using several averaging techniques, and compare these results to an analytical solution.

Analytical Solution

The governing equation for steady-state one-dimensional aquifer flow can be written:

$$\frac{dq}{dx} = 0 \qquad (1)$$

in which q $[L^2/T]$ is volumetric discharge per unit width (Δy). This is a "hydraulic approach" equation in that vertical flux is ignored and (1) reflects integration over the thickness of the layer.

Integrating (1) once we obtain

$$q = \text{constant}$$

and from Darcy's law we recognize

$$q = -KB\frac{dh}{dx} \qquad (2)$$

where K [L/T] is hydraulic conductivity; B[L] is layer thickness; and h[L] is piezometric head.

Integrating (2) assuming K is constant*, we solve for h:

$$\int_1^2 dh = -\frac{q}{K}\int_1^2 \frac{dx}{B} \qquad (3)$$

For a linear varying thickness

$$B(x) = B_1 + \alpha \Delta X$$
$$\Delta X = X - X_1 \qquad (4)$$

Substituting (4) into (3):

$$\int_1^2 dh = -\frac{q}{K}\int_1^2 (B_1 + \alpha X - \alpha X_1)^{-1}\, dx$$

$$\Delta h = -\frac{q}{K\alpha}\left[\ln|B_1+\alpha\Delta X| - \ln|B_1|\right] ; \alpha \neq 0 \qquad (5)$$

in which $\Delta h = h_2 - h_1$. Substituting:

$$\ln|B_1 + \alpha\Delta X| = \ln|B_1| + \ln\left|1 + \frac{\alpha\Delta X}{B_1}\right|$$

into (5) we obtain:

$$\Delta h = -\frac{q}{K\alpha}\left[\ln\left|1 + \frac{\alpha\Delta X}{B_1}\right|\right] ; \quad \alpha \neq 0 \qquad (6)$$

*The following analysis applies equally to a constant thickness layer with linearly varying hydraulic conductivity.

This solution is compared to corresponding solutions from a finite difference technique using averaged interface layer thickness.

Finite Difference Computation

The finite difference representation of flux between 1 and 2 is:

$$q = -K'B'\frac{\Delta h}{\Delta x} \qquad (7)$$

in which K' and B' are the interface values of hydraulic conductivity and layer thickness. Thus the head difference between 1 and 2 is:

$$\Delta h = -\frac{q\,\Delta x}{K'\,B'} \qquad (8)$$

The accuracy of various techniques for computing B' can be investigated by comparing (8), with constant K' = K, to the analytical solution (6).

Harmonic Average

The harmonic average layer thickiness is:

$$B_h' = \frac{2}{\frac{1}{B_1} + \frac{1}{(B_1 + \alpha\Delta x)}} \qquad (9)$$

If α=0, layer thickness is constant, and (9) reduces to $B' = B_1$. Substituting (9) into (8):

$$\Delta h_h = -\frac{q\,\Delta x}{K\,2\,B_1}\left[1 + \frac{1}{1 + \frac{\alpha\Delta x}{B_1}}\right] \qquad (10)$$

The ratio of (10) to (6) can be a relative measure of error. A ratio of 1 is an exact solution with no error. For harmonic average, this ratio is:

$$\frac{\Delta h_h}{\Delta h} = \frac{1}{2}\,\frac{\alpha\Delta x}{B_1}\left(1 + \frac{1}{1 + \frac{\alpha\Delta x}{B_1}}\right)\left(\ln\left|1 + \frac{\alpha\Delta x}{B_1}\right|\right)^{-1} \qquad (11)$$

This ratio is a function of $\alpha\Delta x / B_1$ alone, which is the ratio of thickness change between nodes to thickness at node 1.

Arithmetic Average

The arithmetic average layer thickness is:

$$B'_a = \frac{1}{2}\left(B_1 + B_1 + \alpha \Delta x\right) \qquad (12)$$

Substituting (12) into (8)

$$\Delta h_a = - \frac{2 q \Delta x}{K B_1 \left(2 + \frac{\alpha \Delta x}{B_1}\right)} \qquad (13)$$

The arithmetic solution head difference ratio is

$$\frac{\Delta h_a}{\Delta h} = \frac{2 \alpha \Delta x}{B_1}\left(2 + \frac{\alpha \Delta x}{B_1}\right)^{-1}\left(\ln\left|1 + \frac{\alpha \Delta x}{B_1}\right|\right)^{-1} \qquad (14)$$

Geometric Average

The geometric average layer thickness is

$$B'_g = \left[B_1\left(B_1 + \alpha \Delta x\right)\right]^{1/2} \qquad (15)$$

Substituting (15) into (8)

$$\Delta h_g = - \frac{q}{K B_1 \left(1 + \frac{\alpha \Delta x}{B_1}\right)^{1/2}} \qquad (16)$$

The geometric solution head difference ratio is

$$\frac{\Delta h_g}{\Delta h} = \frac{\alpha \Delta x}{B_1}\left(1 + \frac{\alpha \Delta x}{B_1}\right)^{-\frac{1}{2}}\left(\ln\left|1 + \frac{\alpha \Delta x}{B_1}\right|\right)^{-1} \qquad (17)$$

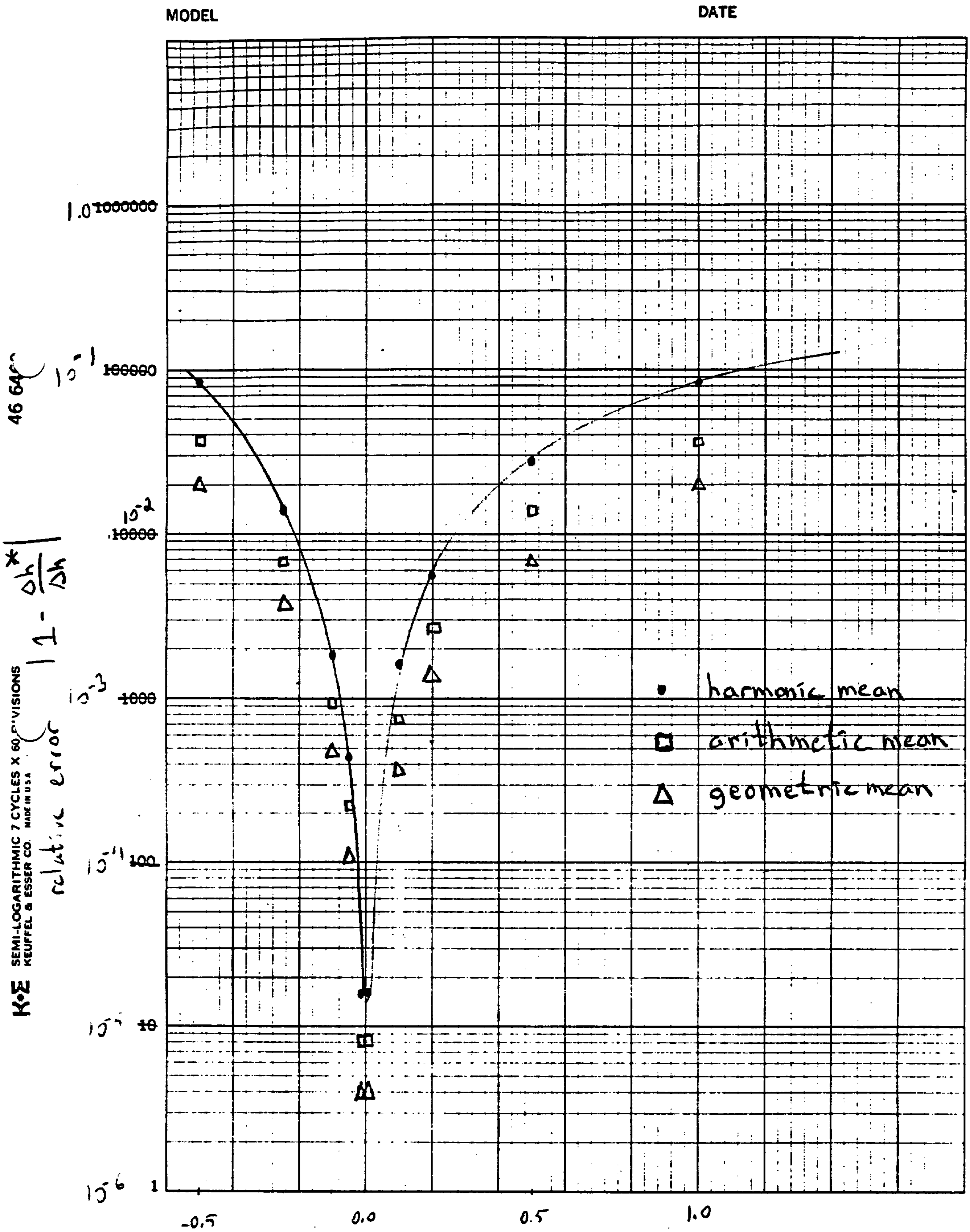
Comparison

The relative accuracy of the harmonic, arithmetic and geometric means in estimating effective interface value are illustrated in Figures 2 and 3. Figure 2 is a semilog plot of relative error versus small relative changes in layer thickness. Relative error is the absolute difference between unity and the ratio of finite difference head change to analytical head change between nodes. The harmonic mean is the least accurate and the geometric is most accurate. For a 50% increase in thickness between nodes ($\alpha \Delta x / B_1 = 0.5$), use of harmonic mean results in an error of about 3%, while arithmetic mean yields about 1.5% error and geometric mean yields about 0.7% error.

Figure 3 illustrate accuracy of the three techniques when hydraulic conductivity changes by orders of magnitude between nodes. The ratio of finite difference head change to analytical head change between nodes is plotted versus the relative change in hydraulic conductivity on a log-log scale. The finite difference head change using harmonic and geometric means is larger than the analytical solution while the head change using arithmetic mean is smaller than analytical. For a three order of magnitude increase in hydraulic conductivity the head difference ratios for the harmonic, arithmetic, and geometric mean techniques are about 70, 0.3, and 4.5, respectively.

If the system flow parameters are conceptualized as varying linearly between nodes, the harmonic mean is the least accurate technique for estimating effective interface values.

Fig. 2 Comparison of averaging techniques - Small changes (A.11)



$\frac{\alpha \Delta X}{B_1}$ relative thickness change

Fig 3 Model head difference error between nodes with linear increase in K. Comparison of averaging techniques. Large changes

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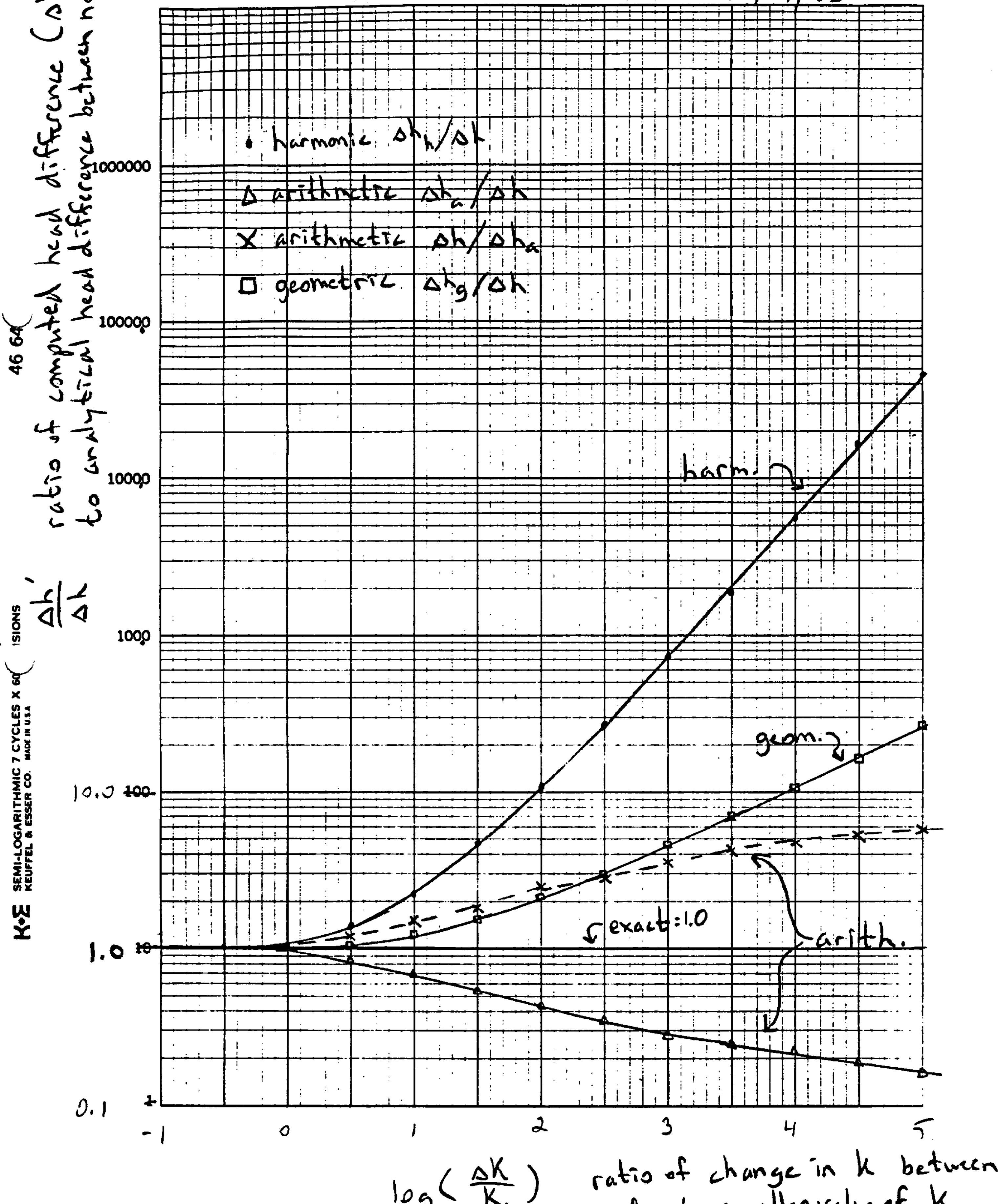

From ~~Appendix~~ Attachment A it is apparent that an averaging function should exist which will replicate the analytical solution exactly. This function is derived below.

Restating Eqn A-6,

$$\Delta h = -\frac{q}{K_1 \alpha}\left[\ln\left|1 + \frac{\alpha \Delta x}{B_1}\right|\right] \qquad (B\text{-}1)$$

and noting that

$$\alpha = \frac{B_2 - B_1}{\Delta x} \qquad \text{and} \qquad \Delta B = B_2 - B_1$$

reduces to

$$\Delta h = \frac{-q\,\Delta x}{K_1\,\Delta B}\left[\ln\left|1 + \frac{\Delta B}{B_1}\right|\right] \qquad (B\text{-}2)$$

The finite difference equation (A-8) using mean values for ~~Δx~~ ΔB is set equal to (B-2) as follows

$$\frac{q\,\Delta x}{K_1\, B^*} = \frac{q\,\Delta x}{K_1\,\Delta B}\left[\ln\left|1 + \frac{\Delta B}{B_1}\right|\right] \qquad (B\text{-}3)$$

Solving for B^*, the effective layer thickness,

$$B^* = \frac{\Delta B}{\ln\left[\left|1 + \frac{\Delta B}{B_1}\right|\right]} \qquad \Delta B \neq 0 \qquad (B\text{-}5)$$

or

$$B^* = \frac{B_2 - B_1}{\ln\left[\left|1 + \frac{B_2 - B_1}{B_1}\right|\right]} \qquad B_2 \neq B_1$$

or

$$B^* = \frac{B_2 - B_1}{\ln\left|B_2/B_1\right|} \qquad B_2 \neq B_1$$