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A critical discussion of numerical models for multiaquifer systems

ISMAEL HERRERA, JEAN PIERRE HENNART and ROBERT YATES
Instituto de Investigaciones en Matematicas Aplicadas y en Sistemas, Universidad Nacional Autonoma de Mexico, Apartado Postal 20-726, *Mexico* 20, *DF, Mexico*
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Leaky aquifers constitute complicated hydrological structures, whose inclusion in numerical models of hydrological systems is difficult, because of their three-dimensional nature. Methods for treating such systems can be classified as fully three-dimensional and quasi-three-dimensional. The latter have clear numerical advantages when applicable. In this paper a critical discussion of existing quasi-three-dimensional models is presented.

INTRODUCTION

When applying mathematical modelling in groundwater hydrology it is frequently necessary to consider multi-aquifer systems. This leads to problems in three spatial dimensions, which involve four independent variables when transient phenomena are considered. Three-dimensional models of groundwater flow systems are available[5,19], but owing to economic considerations, two-dimensional representations when possible, are preferred in most cases[7].

Theories in which the flow is assumed to be horizontal in the aquifers and vertical in the intervening aquitards, are frequently called quasi-three-dimensional. The error introduced in this manner is generally 5% or less[20] which is acceptable for most engineering purposes. Quasi-three-dimensional models result in considerable reductions in computer time as well as in storage requirements, when compared with fully three-dimensional models whose only advantage is their complete generality. Hence, in the critical discussion here presented, attention is restricted to quasi-three-dimensional models.

In order to profit fully from these advantages, it is important to eliminate the vertical coordinate from the governing equations. This was achieved in early work by assuming that leakage is proportional to hydraulic head difference across the aquitard[11,18]; this condition is strictly satisfied in steady state situations, but in transient problems it may be quite inaccurate; it implies for example, neglecting the aquitard storage. Hantush[10] developed a solution for an isolated well that takes storage into account in an approximate manner. Herrera and Figueroa[14] formulated a manner of incorporating Hantush's approximations of the aquitard storage into the governing equations of leaky aquifers and multi-aquifer systems[12], thus allowing the treatment of a greater variety of geometries and boundary conditions. Bredehoeft and Pinder[1] using an analytical solution due to Hanshaw and Bredehoeft[9], developed a semi-analytical procedure to account for the aquitard storage. Fujinawa[8] formulated a finite element model in which a linear approximation of the aquitard response is incorporated.

All the techniques mentioned up to now, for eliminating the z-coordinate from the quasi-three-dimensional models, are of limited applicability. A rigorous and exact procedure for eliminating the vertical coordinate was given by the integro-differential approach. Herrera and Figueroa[14] and Herrera[12] obtained a system of integro-differential equations which is strictly equivalent to the basic equations of motion of the quasi-three-dimensional theory of multiaquifer systems. These equations were developed systematically by Herrera and Rodarte[15]. Later Herrera and Yates[16] and Herrera *et al.*[17] presented a procedure to treat numerically these integro-differential equations efficiently. Herrera and Rodarte[15] established the equivalence between two different series developments for the flow into an aquifer from a neighbouring aquitard produced by a stepwise head change in the aquifer; one of these developments can be recognized as that obtained by Hanshaw and Bredehoeft[9] and incorporated by Bredehoeft and Pinder[1] in their theory. However, it is the alternative series development that is better suited for numerical treatment as it allows the formulation of a method whose accuracy is not restricted[16,17] because it can be made as accurate as desired by properly choosing the truncation of the series expansion of the kernels. The method includes many other approximate models as particular cases. In the light of the integro-differential equations, it is possible to interpret these different approximations as alternative manners of approximating the kernel functions. This allows a systematic development of such models. Corresponding to each approximate theory, a numerical method to treat multiaquifer systems can be developed. Up to date only a few of the many alternatives have been used. For example, Herrera and Figueroa's correspondence principle[14], to our knowledge, has not been applied in spite of being a very simple and numerically convenient manner of accounting approximately for aquitard storage; the range of applicability of this approximation is essentially the same as that of Hantush's[10] large time approximation[13], but it can be applied to inhomogeneous aquifers in arbitrary geometries and subjected to general boundary conditions.

Later, Chorley and Frind[2] developed another method

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of unrestricted applicability, which treats directly the basic equations of motion. An essential feature of this scheme is that the aquitard response is obtained by solving numerically its governing differential equations.

De Marsilly *et al.*[4] have recently published a method which does not present any major difference with the integro-differential equations approach here discussed, except for the fact that it does not incorporate some refinements[16]. Frind[6], has just published a discussion of the memory functions occurring in the integro-differential equations, oriented to numerical applications; this is related with one presented by Herrera. However, Frind concludes that it is not clear whether or not his results lead to an improvement of the original procedure developed by Herrera and Yates[16].

EXISTING QUASI-THREE-DIMENSIONAL MODELS

In this section, we describe Chorley and Frind's model[2] (in what follows, model A), and the integro-differential equations model (in what follows, model B)[16,17,22]; these are as far as we know the only existing ones which can be made as accurate as desired, within the general framework of quasi-three-dimensional models. For the sake of simplicity, we shall consider the system of Fig. 1, although both formalisms apply to multiaquifer systems.

Under the assumption of horizontal flow in the aquifers and vertical flow in the aquitard, the equations of motion are, for a confined aquifer:

$$\frac{\partial}{\partial x}\left[T\frac{\partial s}{\partial x}\right]+\frac{\partial}{\partial y}\left[T\frac{\partial s}{\partial y}\right]=S\frac{\partial s}{\partial t}+Q+q_L \qquad (1)$$

and for a water table aquifer under the Dupuit approximation:

$$\frac{\partial}{\partial x}\left[Kb(s)\frac{\partial s}{\partial x}\right]+\frac{\partial}{\partial y}\left[Kb(s)\frac{\partial s}{\partial y}\right]=S_y\frac{\partial s}{\partial t}+Q+q_L \qquad (1')$$

where q_L is the leakage flux, and the notation is standard in aquifer mechanics. Boundary conditions are of the usual Dirichlet and Neuman type. The aquitards are governed by:

$$\frac{\partial}{\partial z}\left[K'\frac{\partial s'}{\partial z}\right]=S_s'\frac{\partial s'}{\partial t} \qquad (2)$$

In both models A and B, a finite element solution for the aquifers is formulated in the usual way. The main difference between them resides in the treatment of the flux term q_L due to leakage in equations (1) and (1'), which by Darcy's law is the product of the permeability K' and the vertical gradient of the aquitard drawdown s'.

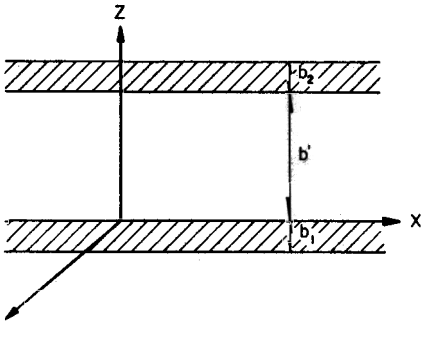

Figure 1

In model A, the aquitard equation remains within the final set of equations, which consists of three partial differential equations of parabolic type, one for the aquitard and two for the adjacent aquifers. For the aquitards a string of linear elements is used by Chorley and Frind[2]. Nothing is assumed with respect to the vertical variation of the aquitard permeability which can be arbitrary. However, the explicit consideration of the aquitard equation introduces a direct coupling between the aquifers and aquitard equations via the leakage terms q_L which leads to an iterative method of solution: the aquifers and aquitard are solved alternatively at each time step, in a way that becomes more complex as more than two aquifers are considered, even when a sequential solution procedure is adopted.

In model B, the aquitard equation is integrated out leading to a set of two integro-differential equations, one for each aquifer, where the flux terms become convolutions with memory and influence functions:

$$q_{L_1}=K'\left.\frac{\partial s'}{\partial z}\right|_{z=0}=K'\left\{\int_0 f(t'-\tau)\frac{\partial s_1}{\partial t'}(\tau)\mathrm{d}\tau + \int_0 h(t'-\tau)\frac{\partial s_2}{\partial t'}(\tau)\mathrm{d}\tau\right\} \qquad (3)$$

and a similar expression for q_{L_2}. Here $t'=\alpha' t/b'$, while[15]

$$f(t')=1+2\sum_{n=1} \mathrm{e}^{-n^2\pi^2} =\frac{1}{(\pi t')^{1/2}}\left(1+2\sum_{n=1}^{\infty}\mathrm{e}^{-n^2/t'}\right) \qquad (4)$$

and

$$h(t')=1+2\sum_{n=1} -1)^n\mathrm{e}^{-n^2\pi^2 t'} \qquad (5)$$

This procedure does not introduce any approximation as long as the aquitard permeability K' is taken to be constant vertically across the aquitard. If vertical variability is permitted, the same procedure remains valid under the assumption that a vertically averaged K' can be obtained. In equation (3) the first and second terms in the right-hand side represent the influence of aquifers 1 and 2 on aquifer 1, respectively. Equation (4) represents an identity between two alternative expressions for function f. The second of these was used by Bredehoeft and Pinder[1] to formulate an approximate method of solution. The first one has numerical advantages which lead to the method of unrestricted accuracy discussed here. In this scheme, the memory and influence terms are approximated by a truncation of their exponential series done in such a way as to preserve the values of their integrals. This conservation of mass helps to avoid systematic errors. The resulting equations are directly solved by any standard finite element technique as for model A. These equations, owing to the shape of the influence function h, may be regarded as uncoupled which eliminates the need for an iterative procedure. Furthermore, the convolution in-

tegrals can be evaluated at each time step by a simple updating procedure, which is independent of any reference time and does not involve past history; this is possible because of the exponential nature of the series approximations[16]. Finally, the drawdown in the aquitard need not be calculated unless it is required at some time t', in which case it can be evaluated simply in terms of the values in the adjacent aquifers and of auxiliary terms which occur in the calculation:

$$s'(z,\,t)=s_1(t')(1-\zeta)+s_2(t')\zeta-$$

$$2\sum_{n=1}^{N'}[d_{1n}(t')-(-1)^n d_{2n}(t')]\frac{\sin n\pi\zeta}{n\pi} \qquad (6)$$

If $N'=N$, $d_{\gamma n}(t')$ is already available; wnen $N'>N$ the additional terms can be computed simultaneously without any recalculation[22].

In their original paper, Herrera and Yates[16] formulated the method for homogeneous aquifers. By an extension of their procedure this restriction has been eliminated[22] and general heterogeneous aquifers can be treated thanks to a lumping technique using reduced integration[23]. This presents several additional advantages such as increased stability of the algorithm and simplicity in the treatment of general boundary conditions, as well as the calculation of source terms. Finally, the treatment of water table aquifers under Dupuit's assumption, can be incorporated using the standard techniques for such systems[3].

COMPARISON BETWEEN EXISTING QUASI-THREE-DIMENSIONAL MODELS

One of the main points in comparing the two models lies in the treatment of the aquitard: in model A, even if the drawdown in the aquitard is not explicitly required, the aquitard must be correctly discretized to avoid introducing numerical errors in the aquifer calculation, especially because the aquifer-aquitard coupling occurs through the leakage flux across the aquifer–aquitard interfaces. This flux depends on the vertical gradient in the aquitard by Darcy's law, which means that special care must be exercised to evaluate the aquitard drawdown since errors associated with gradients are typically greater than errors associated with values. In point of fact, a relatively involved procedure is used in model A to select the grid in the aquitard. Moreover, the mesh size in the aquitard will depend on both its thickness and permeability. In model B, the aquitard flux is analytically incorporated into the original equations: therefore it is not required to solve for the values of the aquitard. Rather these values can be derived as explained in the previous section. It is interesting to note that increased complexities in model A due to the aquitard discretization are reflected in model B through the number of series terms that are required for comparable accuracies. In model B, for given values of time, aquifers and aquitard characteristics, and prescribed accuracy, it is possible to predetermine and dynamically adapt the number of terms to be retained in the series approximations. These terms do not significantly increase the computational costs, because they appear as source terms, whose evaluation is considerably simplified by the lumping procedure mentioned earlier. In both models, arbitrary boundary and initial conditions, as well as space and time dependent source terms, can be incorporated.

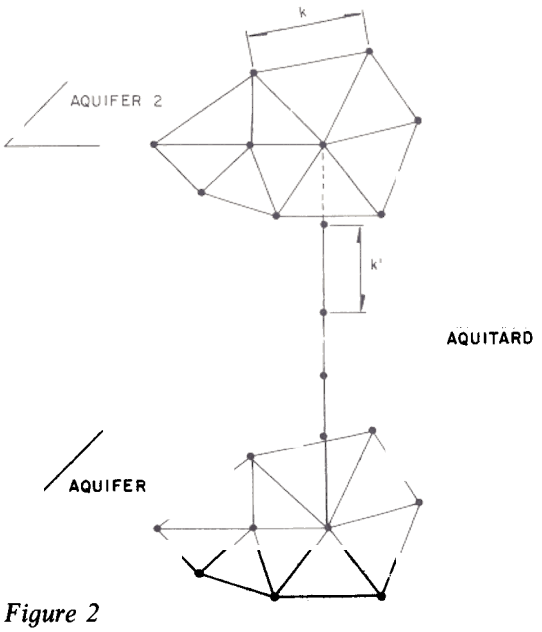

Figure 2

Moreover, they are independent of the reference time chosen.

A rough comparison in computational costs between models A and B can be carried out as follows for a general system of N aquifers, separated by $(N-1)$ aquitards, the Nth aquifer being confined. Suppose that all the aquifers are discretized by 2D finite elements of diameter k, while the aquitards are discretized by 1D finite elements of size k' (Fig. 2). If, for instance, linear elements were used, the numbers of unknowns (n for the aquifers, n' for the aquitards) as well as the half bandwidths (w for the aquifers, w' for the aquitards) of the resulting algebraic systems would be given by

$$n\sim k^{-2}, \qquad w\sim k^{-1} \qquad (7)$$

and

$$n'\sim(k')^{-1}, \qquad w'=2 \qquad (8)$$

so that the corresponding number of arithmetic operations for a matrix factorization (F for the aquifers, F' for the aquitards) and for a solution with a given second member (S for the aquifers, S' for the aquitards) are[21]

$$F=\tfrac{1}{2}nw^2\sim\tfrac{1}{2}k^{-4}, \qquad S=2nw\sim 2k^{-3} \qquad (9)$$

and

$$F'=\tfrac{1}{2}n'w'^2\sim 2k'^{-1}, \qquad S'=2n'w'\sim 4k'^{-1}. \qquad (10)$$

If we assume that the bulk of the computational effort consists of the repeated solution of the algebraic systems at each time step and of the matrix factorizations in the first time interval and moreover, that model A requires l iterations at each time step, the total computational costs in numbers of arithmetic operations for models A and B to be denoted by C_A and C_B respectively, may be evaluated supposing that m time steps in total are performed. In this manner, we obtain in the general heterogeneous case:

$$C_A=NF+(N-1)k^{-2}F'+$$

$$lm(NS+(N-1)k^{-2}S') \qquad (11)$$

because there are k^{-2} strings of linear elements across the aquitards in model A. Similarly:

$$C_B = NF + mNS \tag{12}$$

If a fully 3D model (hereafter model C) is included in the comparison, the corresponding computational costs are:

$$C_C = F + mS \tag{13}$$

where

$$F = \tfrac{1}{2}nw^2, \qquad S = 2nw \tag{14}$$

with

$$n \sim k^{-2}(N-1)k'^{-1}, \quad w = \min(k^{-1}, (N-1)k'^{-1}) \tag{15}$$

A comparison of computational costs based on matrix factorizations and solutions is, of course, not entirely satisfactory. In model A, for instance, it does not take into account the fact that the iterative procedure which successively solves for the aquifers and the aquitards becomes more complex as more than two aquifers are considered, even when the strongest coupling between neighbouring aquifers is taken into account, leading eventually to a sequential solution procedure. In model B, on the other hand, this comparison does not consider the successive updating of the memory and influence terms in each aquifer equation. With these restrictions in mind, it should, however, be clear that such a comparison is at least qualitatively correct and gives a fairly good idea on how these models would compare in realistic situations.

If, for example, the scaling $m \sim k^{-1} \sim (k')^{-1}$ is chosen which is consistent with a Crank–Nicholson time discretization scheme where the space and time errors are expected to be both of second order, it is easy to verify that in the absence of a water table aquifer

$$C_A = (0.5N + 6Nl - 4l)m^4 + 2(N-1)m^3 \tag{16}$$

$$C_B = 2.5\, Nm^4$$

$$C_C = 0.5m^5 + 2m^4$$

From these estimations of computational costs, it is clear that model C is not competitive with either model A or model B. This conclusion is, however, based on the assumption that even with model C all the matrix operations are direct, as opposed to iterative; actual implementations of model C are or at least should be iterative. In the following, model C will therefore not be included in the comparison. From (16) and (17), we get:

$$C_A/C_B = \frac{0.5N + 6Nl - 4l}{2.5N} + \frac{1}{m}\,\frac{2(N-1)}{2.5N} \tag{19}$$

so that if five iterations are assumed per time step ($l = 5$) with model A[2], we obtain

$$C_A/C_B \sim 8.2 \qquad \text{for } N = 2 \tag{20}$$

while

$$C_A/C_B \to 12.2 \qquad \text{as } N \to \infty \tag{21}$$

showing that the computational costs can be roughly reduced by an order of magnitude when model B is used instead of model A. It is easy to check that these numbers 8.2 and 12.2 would become 10 and 15 respectively, if a scaling $m \sim k^{-2} \sim (k')^{-2}$ were chosen. Such a scaling is consistent with a Backward Euler time discretization scheme where the space errors are still of second order, but the time errors are only of first order.

It can be seen that the above results are essentially not altered when homogeneous aquifers are considered.

If the upper aquifer is a water table one, the factorization has to be performed at each time step for this aquifer and the corresponding computational costs become

$$C_A = (N - \ + m)F + (N-1)k^{-2}F' + lm(NS + (N-1)k^{-2}S' \tag{22}$$

and

$$C_B = (N - 1 + m)F + mNS \tag{23}$$

The mF term appearing in both expressions is presumably dominant if m is large, with the consequence that C_A/C_B will be correspondingly reduced. This is natural because it reflects the fact that most of the computational effort is required by the phreatic aquifer which is not linear; thus, the simplification achieved in the treatment of the aquitard is relatively less important.

Of course, model B is applicable under the assumption that K' is constant vertically or can be suitably averaged in that direction. This seems to be a quite frequent situation in practice, in particular when the field data are scattered and do not provide more than a reasonable average value of K'. On the other hand, if a sufficiently precise vertical variation of K' is known, which is too irregular to lend itself to some averaging procedure, an extension of model B[22] to arbitrarily inhomogeneous aquitards that has just been developed, can be used.

The basic computational costs (and also the memory requirements) are given in Table 1. As an illustration of

Table 1. *Basic computational costs and memory requirements**

	Model A	Model B
Number of unknowns		
n (*Aqf*)	$\sim k^{-2}$	$\sim k^{-2}$
n' (*Aqt*)	$\sim (k')^{-1}$	–
Half bandwidths		
w (*Aqf*)	$\sim k^{-1}$	$\sim k^{-1}$
w' (*Aqt*)	2	–
Memory requirement for *Aqf* & *Aqt* matrix storage	$\sim Nk^{-3} + 2(N-1)(k')^{-1}$	$\sim Nk^{-3}$
Matrix factorization		
F (*Aqf*)	$\sim \frac{1}{2}k^{-4}$	$\sim \frac{1}{2}k^{-4}$
F' (*Aqt*)	$\sim 2(k')^{-1}$	
Solution		
S (*Aqf*)	$\sim 2k^{-3}$	$\sim 2k^{-3}$
S' (*Aqt*)	$\sim 4(k')^{-1}$	–

* *Aqf* = Aquifer, *Aqt* = Aquitard

*Table 2. Computational costs ratios C_A/C_B for some possible situations**

Situation	Space-time mesh**	C_A/C_B
2 aquifers & 1 aquitard no water-table aquifer	10 x 10 x 10 x 10 40 x 40 x 40 x 40 40 x 40 x 40 x 160	
10 aquifers & 9 aquitards no water-table aquifer	10 x 10 x 10 x 10 40 x 40 x 40 x 40 40 x 40 x 40 x 160	
2 aquifers & 1 aquitard with water-table aquifer	10 x 10 x 10 x 10 40 x 40 x 40 x 40 40 x 40 x 40 x 160	
10 aquifers & 9 aquitards with water-table aquifer	10 x 10 x 10 x 10 40 x 40 x 40 x 40 40 x 40 x 40 x 160	

* For model A, five iterations are assumed per time step ($l = 5$)– See Chorley & Frind[2]

** Defined as 'number of intervals in the x direction × number of intervals in the y direction × number of intervals in the z direction × number of time steps'.

the above discussion, Table 2 exhibits some numerical estimations of C_A/C_B in different possible situations.

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