INFLUENCE OF BOUNDARY CONDITIONS ON TRACER DISPERSION IN AN AQUIFER

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Abstract

Dispersivity is often assumed to be independent of the flow boundary conditions. As dispersion of a plume is a consequence of Darcy's velocity fluctuations, boundary conditions should influence this process and, possibly, affect the dispersivities defined far from the boundaries.

In this work, we analyze, by means of Monte-Carlo simulations, the influence of different types of boundary conditions on flow and transport statistical quantities in a bidimensional aquifer. Results show that boundary conditions have a short range influence on velocity mean and variances, and a long range influence on transport. For instance, transverse dispersivity is very sensitive to the nature of lateral boundary conditions : for an imposed head the range of influence is at least eight correlation lengths. On the basis of these results, dispersivity in bidimensional aquifers appears to be dependent of boundary conditions in a zone, along the boundaries, of rather large extent.

INTRODUCTION

Contaminant transport in heterogeneous aquifers is usually modeled by an advection diffusion dispersion equation. The dispersivities are often assumed to be independent of the flow boundary conditions. Whatever the modeling approach, classical or stochastic, the dispersion process is a consequence of the Darcy velocity fluctuations. Therefore, boundary conditions potentially influence this process and, possibly, affect the dispersivities defined far from these boundaries.

Head boundaries set head fluctuation to zero while flux boundaries annuls one component of Darcy's velocity. By constraining different variables, different type of boundary do not produce the same flows in heterogeneous media. For instance, a mean uniform flow can be generated by fixed head up- and down-stream, and impervious lateral borders. These latter borders with fixed linear head produce the same average flow, but are not impervious anymore. It is clear that transport of a plume or of a particle should also be affected.

If this phenomenon is well understood and accepted, the question of its importance and its range in 2D-aquifers has been partially studied. Studies have shown analytically or by Monte-Carlo simulations that log-transmissivity-head cross-correlations C_{yh} and head variogram γ_{hh} are stationary beyond a few correlation lengths λ from the borders [7] [8] [6] [4], but head variance is strongly determined by the boundary conditions, all over the area they delimit, in a log-like variation [2] [4]. Head statistics can then never be considered stationary, except for very large areas. Incidence on velocity is then expected to have the same extent, but this topic is less richly described in the literature. Bellin [1] observed a very clear impact of fixed-flux boundaries on velocity variance. This effect, however, is located in the vicinity of the borders, no more than 3λ away from them. The influence of other types of boundary was not investigated, nor was the study extended to velocity correlations, which are the sources of dispersion. Therefore, it can not be concluded that there should be a "boundary free" zone where head, velocity or transport would behave, from the stochastic point of view, like in an infinite domain.

The purpose of this study is to understand and to investigate by Monte-Carlo simulations if and how dispersion in a uniform mean flow is affected by boundaries, especially lateral boundaries. Simulations were made with the code CASTEM 2000. They rely on the resolution of the flow equations by Mixed-Hybrid Finite Element method [5]. Transmissivity realizations were generated by the matrix decomposition method for an exponential transmissivity correlation, and transport was simulated by particle tracking technique.

In this work, we analyze, by means of Monte-Carlo simulations, the influence of different types of boundary conditions on flow and transport statistical quantities in a bidimensional aquifer. These are the means and variances of Darcy's velocity and particle position. The velocity first two moments are first analyzed analytically under the linearized model.

1 FLOW STATISTICS IN THE VICINITY OF BOUNDARIES

1.1 Theoretical framework

Let axis 1 be the direction of the uniform mean flow, and let us call Y the log-transmissivity, split into a mean $<Y>$ and a random fluctuation y. Y is supposed stationary so that the log-transmissivity correlation depends only on the separation $\vec{r}$: $C_{yy}(\vec{r}) =< y(\vec{x})y(\vec{x}+\vec{r})>= exp(-r/\lambda)$. Head is noted $H =<H> +h$ and Darcy's Velocity is written $\vec{U} =<\vec{U}> +\vec{u}$.

There are four types of boundary : fixed head or fixed flux on lateral - parallel to the mean flow - or longitudinal - perpendicular to the mean flow - borders. In each case, only one variable fluctuation is set to zero : either $h = 0$ or $\vec{u}\cdot\vec{n} = 0$ (where $\vec{n}$ is a unitary vector normal to the boundary) respectively.

The linearized model [3] gives expressions of Darcy's velocity mean and fluctuation :

$$<\vec{U}>= -T_G\left[(1+\sigma_Y^2/2)\vec{J}_0+ <y\vec{\nabla}h> +\vec{\nabla} <H^{(2)}>\right] \quad (1)$$

$$\vec{u} = -T_G\left[y\vec{J}_0 + \vec{\nabla}h\right] \quad (2)$$

given the equations on first order head fluctuations $h = H^{(1)}$ and second order head $H^{(2)}$:

$$\Delta h = -\vec{J}_0\cdot\vec{\nabla}y \quad \text{with the proper boundary conditions} \quad (3)$$

$$\Delta H^{(2)} = -\vec{\nabla}h\cdot\vec{\nabla}y \quad , H^{(2)} \text{ equals zero on the boundaries} \quad (4)$$

The numbers in parenthesis are the σ_y orders in the linearized development (written till order 2). The zeroth order head gradient has been written $\vec{J_0}$, and the geometric mean of transmissivity T_G. We define also the zeroth order mean velocity $U_0 = -T_G J_0$.

Each of these expressions takes different forms depending on the boundary conditions (from eq. (2)) :
- a fixed head longitudinal boundary sets $h = 0$ and $\partial_2 h = 0$, so $u_2 = 0$,
- a fixed flux longitudinal boundary sets $u_1 = 0$, so $\partial_1 h = -y\, J_0$,
- a fixed head lateral boundary sets $h = 0$ and $\partial_1 h = 0$, so $u_1 = y\, U_0$,
- an impervious lateral boundary sets $u_2 = 0$, so $\partial_2 h = 0$.

Mean Velocity

The analytical steps in the calculation of mean velocity are the determination of $< y\vec{\nabla}h>$ from (3) and of $\vec{\nabla} <H^{(2)}>$ from (4), taking advantage of the symmetries generated by the boundaries. This has been made for lateral boundaries only. In the following, the origin is taken on the boundary itself.

Resolution of eq. (3) with head lateral boundary can be done using a composed Green function $G(\vec{x}, \vec{x}') = G^{\infty}(x_1, x_2, x_1', x_2') - G^{\infty}(x_1, x_2, x_1', -x_2')$, where G^{∞} is the Green function for the laplacian in an infinite 2D medium. This case can be described by a fictitious infinite domain where y would be anti-symmetrical in relation to the boundary. Multiplying (3) by $h(\vec{x}')$ and then taking ensemble mean gives :

$$<y(\vec{x})h(\vec{x'})> = -J_0 \int_{\vec{r}\in \text{half plane}} G(\vec{x}', \vec{x}+\vec{r})\partial_{r1} C_{yy}(\vec{r}) d\vec{r} \tag{5}$$

The particular symmetry of G associated to the parity of $C_{yy}(\vec{r})$ is such that this integral is null when $x_1 = x_1'$, whatever x_2 and x_2', so that $< y(x_1, x_2)\, \partial_{x2} h(x_1, x_2) >= 0$ too. Furthermore, due to the nature of the boundary, $\partial_1 h(x_1, 0) = 0$. So :

$$<y\vec{\nabla}h>\ (x_1, 0) = \vec{0} \tag{6}$$

Moreover, $H^{(2)}$ being null on the boundary, $\partial_{x1}<H^{(2)}>= 0$. Mean longitudinal velocity in the vicinity of a head lateral boundary, expressed by (1), has then the following form :

$$<U_1>\ (x_1, 0) = (1 + \sigma_y^2\, /\, 2)\ U_0 \tag{7}$$

Mean velocity should then be increased by the proximity of head lateral boundaries, with a magnitude varying linearly with log-transmissivity variance. The range of the influence, however, is not determined a priori.

Fixed-flux lateral boundary does not affect mean velocity, because this situation corresponds to a fictitious infinite domain where y would be symmetrical in relation to the boundary. In this case, eq. (5) is identical to the expression of C_{yh} in an unbounded domain. $H^{(2)}$, $<y\vec{\nabla}h>$ and finally $<\vec{U}>$ are then unchanged.

Velocity variances

Velocity variances on boundaries are obtained directly from eq. (2). Some of them are expressed in relation to head derivative standard-deviation on the boundary. Those

latter were not analytically calculated. It has been found that :
- for fixed head longitudinal boundary, $\sigma_{u1} = T_G\, \sigma_{\partial_{x1}h}(0, x_2)$ and $\sigma_{u2} = 0$
- for fixed flux longitudinal boundary, $\sigma_{u1} = 0$ and $\sigma_{u2} = \sigma_y U_0$,
- for impervious lateral boundary, $\sigma_{u1} = T_G\, \sigma_{\partial_{x1}h}(x_1, 0)$ and $\sigma_{u2} = 0$
- for head lateral boundary, $\sigma_{u1} = \sigma_y U_0$ and $\sigma_{u2} = T_G\, \sigma_{\partial_{x2}h}(x_1, 0)$

1.2 Monte-Carlo simulations

Four values of σ_y have been investigated : 0.1, 0.5, 1.0 and 1.5. The number of realizations necessary to reach a satisfactory convergence were made. The grid refinement is $\lambda/4$ on a $21\lambda \times 13\lambda$ wide area. Simulations have been performed for the two different lateral boundaries with fixed head on the in-flow and the out-flow borders. Results are summarized in table 1.

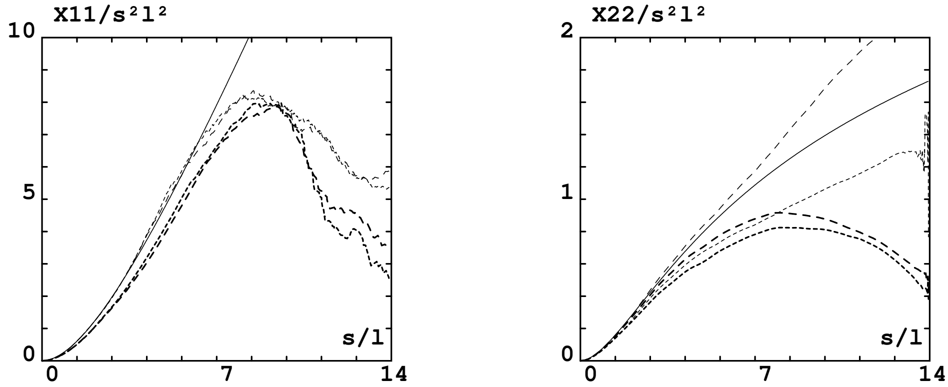
Type of boundary	Lateral, head	Lateral, flux	Long., head	Range for all types
Effect on h	$\longrightarrow 0$	high	$\longrightarrow 0$	everywhere
Effect on $<U_1>$	$\times(1 + \sigma_y^2 / 2)$	slight decrease	-	4λ
Effect on σ_{u1}	strong increase	-	strong increase	3λ
Effect on σ_{u2}	strong increase	$\longrightarrow 0$	$\longrightarrow 0$	3λ

Table 1: Effect and range of boundaries in a uniform flow

Detailed values are not shown, but the simulated increase of $<U_1>$ in the vicinity of a fixed-head lateral boundary is exactly the one predicted by eq. (7) except for σ_y=1.5 (the linearized model usually requires $\sigma_y < 1$). The fit is not as good for longitudinal velocity variance increase near the same boundary. An overestimation of no more than 25% is observed. The results show that velocity variability tends to zero where expected, and increase significantly otherwise. Symmetrically, studies of Dagan [2] and Osnes [4] showed how head fluctuations tend to zero on fixed-head boundaries but increase near impervious lines. In any case, the range of the influence of the boundaries on mean and variances of velocity does not exceed a few correlation lengths. To this point, nothing can be said on how, and how far, can velocity correlations be affected by the boundaries.

2 INFLUENCE OF LATERAL BOUNDARIES ON TRANSPORT IN A UNIFORM FLOW

The influence of the type of lateral boundaries on transport has been studied by Monte-Carlo simulations. We investigate here the particle displacement variances in a uniform flow generated in a 17λ square medium discretized $\lambda/4$. From 800 up to 2000 realizations were performed for each value of σ_y investigated.



(a) Longitudinal (X_{11}) (b) Transverse (X_{22})

Figure 1: Normalized displacement variances functions of dimensionless abscissa s/λ for different boundary conditions : longitudinal head (thin) or flux (bold) conditions, and lateral head (small dashes) or flux (long dashes) boundaries.

We present the position variances as functions of mean travel distance s, of a particle released 3λ from the up-stream border, on the symmetry axis of the medium. Results are quite similar for the four values of σ_y. For the sake of clarity, X_{11} is presented with σ_y=1, and X_{22} with σ_y=0.1 (See Figure 2). Longitudinal dispersion seems not to be affected by lateral boundaries, nor by head longitudinal boundaries ; but fixed-flux longitudinal boundaries induce a significant, though light, decrease of X_{11}. On the other hand, transverse dispersion is clearly dependent on the nature of all four boundaries. Lateral flux boundaries increase X_{22} while lateral head boundaries lower it. After a travel distance of only 7λ, the plume is no more than 0.3λ wide, so still about 8λ away from the lateral borders, but the difference has already got up to 20%. Moreover, X_{22} seems extremely sensitive to longitudinal flux boundaries.

These results suggest that velocity correlations are affected on a very long range (more than 10 λ like other not included calculations showed), while velocity variances are not affected on more than a few λ. Thus, velocity correlation lengths for longitudinal separations seem to be affected by the boundaries on long distances. Within this assumption, transverse velocity correlation length would decrease in the vicinity of a head lateral or flux longitudinal boundary, and increase in the vicinity of a flux lateral boundary. The explanation according to which effective log-transmissivity correlation length doubles near a fixed-flux boundary due to the fictitious symmetry of Y relatively to it, is not pertinent. If the boundary is parallel to the mean flow, then only correlation length for transverse separations is concerned ; and if the boundary is orthogonal to the mean flow, an increase of longitudinal position variance should be observed, which is not the case. The same remark applies to head boundaries. So the observed influence of boundaries on particle position variances remains unexplained, yet indubitable.

3 CONCLUSION

It is commonly accepted that boundaries affect flow and transport in their vicinity. That is why every modeler chooses, somewhat arbitrarily or on the strength of studies not plainly devoted to the topic, an area that he thinks is "boundary free". It has been showed here that boundaries determine flow and transport in a very wide area, at least 10 log-transmissivity correlation lengths away from them. For instance, with lateral boundaries 8λ away from the release point, itself 3λ from the in-flow boundary, the differences in position variances go up to 30% after only 7λ traveled. Longitudinal boundaries exert the more important influence on transport. The influence of transverse boundaries is also certain, though limited to transverse dispersion. This could not be expected on the basis of velocity mean and variances, which reach their infinite-domain values after a short distance. Velocity correlation lengths could be responsible of the effect of boundaries on transport, by being affected on very long ranges. Other explanations could be suggested, like high-order effect not included in the linearized model used here. More analytical research are necessary to understand the long-range effect of boundaries on transport.

From a practical point of view, it must be understood that, unless boundaries are very far apart, they take a full part in the modelization and should be subject to a careful choice. Real field boundaries should be preferred, and if not available, boundary effects should be kept in mind when interpreting results. Finally, the nature of boundaries might be of critical importance in other types of flow, like single or multi-pumping, where the nature (fixed draw-downs or fixed pumping rates) of the wells must be chosen.

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