Tracers and Modelling in Hydrogeology (Proceedings of the TraM'2000 Conference held at Liège, Belgium, May 2000). IAHS Publ. no. 262, 2000.

Modelling the injection of a tracer in a well: a new mathematical and numerical approach

SERGE BROUYÈRE

Laboratory of Engineering Geology, Geophysical Prospecting and Hydrogeology, University of Liège, Bâtiment B19, Sart Tilman, B-4000 Liège, Belgium

e-mail: sbrouyer@lgih.ulg.ac.be

Abstract A new mathematical approach is proposed to model the injection of a tracer in a well for field tracer tests. It is based on the water and tracer mass budget integrated over the injection well, for the different injection steps (tracer injection, water flush and tracer behaviour after the injection). This physical approach deals with well-bore mixing and dilution effects, local distortion of the flow field around the injection well, back-diffusion of the tracer in the injection well after the injection, and tracer capture in the well bore. A numerical solution (finite differences over time) is proposed and implemented in a three-dimensional finite element flow and transport simulator (SUFT3D). A radially converging tracer test is computed to illustrate the adequacy and usefulness of this new mathematical concept to model field results.

INTRODUCTION

Tracer tests are frequently used to assess field aquifer transport properties but usually little attention is paid to the physical and mathematical representation of the injection process in the well. In fact, many physical factors can cause the tracer entry function to depart from theoretical injection profiles (Dirac or step functions), leading to incorrect interpretation of the test. A new mathematical and numerical approach is proposed to model the injection process and the complex well–aquifer interaction more accurately and physically.

MAIN INFLUENCING FACTORS

Injection duration and flow rates can play a significant role on tracer test results (Guvanasen & Guvanasen, 1987; Brouyère & Rentier, 1997) but these are "external" factors, under the control of the experimenter. Thus, they are less problematic. Other factors related to the aquifer properties and test site equipment are more difficult to control and to deal with.

First, a dilution of the tracer occurs with the water present in the well. This can result in lower recovery peaks at pumping wells (Novakowski, 1992; Moench, 1995). This mixing effect is more pronounced for large or deep-drilled wells containing a large volume of water. The dilution is expressed by the ratio of the injected tracer water (V_{in}) and the well water (V_w) volumes.

Second, according to local hydraulic properties (well equipment, aquifer material compaction around the well, etc.), a distortion of the flow field can be observed close to the well (Drost *et al.*, 1968; Klotz *et al.*, 1979). This effect is usually considered through a lumping distortion coefficient (α_w) expressing the ratio between theoretical and actual water flow rates crossing the well section orthogonal to the main flow direction. Provided that the hydraulic characteristics of the well and surrounding aquifer are known, the flow distortion coefficient can be evaluated (Drost *et al.*, 1968; Bidaux & Tsang, 1991).

Finally, water fluxes between the well and the aquifer are often supposed to be uniformly distributed along the screens. The heterogeneous nature of aquifer materials can result in a variation of aquifer conductivity along the screens, resulting in a non-uniform distribution of injected water fluxes along the well. The highest fluxes are encountered at the levels with the highest conductivity (e.g. fractures, well-sorted gravels).

GOVERNING EQUATIONS

The model is based on the concept of mass conservation (water and solute) integrated over the well volume. Flux terms account for the different possible exchanges between the well and its environment (Fig. 1). The well radius is r_w (L) and the length of the water column in the well is h_w (L). Exchanging fluxes (L T^{-3}) are the injected water flow rate Q_{in}, the transit water flow rate Q_t crossing the well at the level of the screens (due to the natural motion of water in the aquifer), and the water flow rate Q_{out} leaving the well through the screens. Concentration terms (M L^{-3}) in the different fluxes are respectively: C_{in}, C_t, C_{out}. The concentration in the well C_w (M L^{-3}) is supposed to be homogeneous (this can be assured by a water circulation in the well).

If density effects are neglected, the expression of water conservation can be written:

$$\frac{\partial V_w(t)}{\partial t} = \pi r_w^2 \frac{\partial h_w}{\partial t} = Q_{in}(t) + Q_t(t) - Q_{out}(t) \tag{1}$$

where $V_w = \pi r_w^2 h_w$ is the volume of water in the well at time t.

The equation of mass conservation applied to the tracer is:

$$\frac{\partial M_t}{\partial t} = \frac{\partial}{\partial t}(V_w C_w) = \pi r_w^2 \left(C_w \frac{\partial h_w}{\partial t} + h_w \frac{\partial C_w}{\partial t} \right) = Q_{in} C_{in} + Q_t C_t - Q_{out} C_{out} \tag{2}$$

where M_t is the mass of tracer injected.

Grouping the two mass conservation equations and supposing that the tracer leaves the well at the concentration in the well ($C_{out} = C_w$) provides the general form of the model:

$$\pi r_w^2 h_w \frac{\partial C_w}{\partial t} = Q_{in}(C_{in} - C_w) + Q_t(C_t - C_w) \tag{3}$$

Evaluation of the transit flow rate Q_t

The transit flow rate Q_t plays a role by diluting the tracer and rinsing the well or, on the contrary by carrying some tracer which migrates back into the well. In natural flow conditions, Q_t can be evaluated by the following expression:

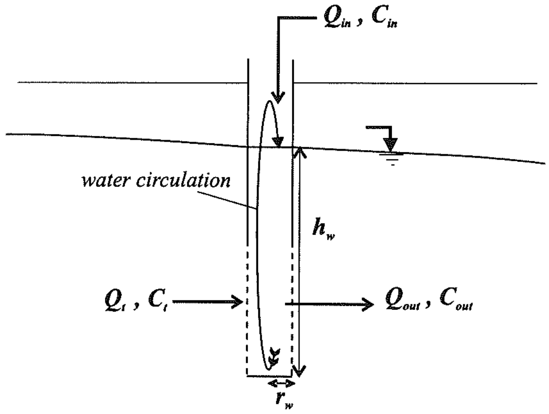

Fig. 1 Schematic representation of the well: the aquifer system and exchanged fluxes.

$$Q_t = \alpha_w v_d S_w \tag{4}$$

In this expression, v_d is the Darcy velocity (L T^{-1}) in the aquifer close to the well, S_w the well cross-section orthogonal to the main flow direction, and α_w the well distortion coefficient.

When water is injected in the well, Q_t is modified and a more general expression has to be evaluated. An analytical formulation has been deduced from the Bideaux & Tsang (1991) potential theory (details not included), providing a continuous variation of Q_t between zero (when Q_{in} is high) and Q_{tmax} (when $Q_{in} = 0$):

If $Q_{in} > Q_{cr}$ $\quad Q_t = 0 \quad$ and $\quad Q_{out} = Q_{in}$ (5)

If $Q_{in} < Q_{cr}$ $\quad Q_t = 2 r_w e V_w \sin\left(\arccos Q^*\right) - \dfrac{Q_{in}}{2\pi}\left(2 \arccos Q^*\right) \quad$ and $\quad Q_{out} = Q_{in} + Q_t$

$Q^* = Q_{in} / Q_{cr}$ where $Q_{cr} = 2\pi e r_w \alpha_w v_d$ is a critical injection rate that exactly cancels the transit flow rate Q_t ($Q_{cr} = \pi Q_t \neq Q_t$).

Equation (5) implies that all fluxes are at equilibrium. This can be justified by the fact that at the scale of the injection well a steady state regime is reached almost instantaneously.

Transit flux concentrations (C_t)

Due to important concentration variations around the well, the evaluation of the transit flux concentration is not easy. A lumped solution is proposed: the well mass outflux is proportional to the concentration C_w in the well during the injection and to the well–aquifer concentration gradient ($C_w - C_{aq}$) when the injection and the flush are finished.

NUMERICAL MODELLING

For flow computation, injection and pumping wells are represented by one dimensional elements with a high axial conductivity and modified storage coefficient

(Sudicky *et al.*, 1995). If n_w nodes connect the well and the aquifer, the flow computation results in a "natural" splitting of the different flow rates Q_{in}, Q_{out} and Q_t into n_w components, according to the local hydrodynamic properties of the aquifer:

$$Q_{in}=\sum_{K=1}^{n_w} q_{in}^K, \qquad Q_{out}=\sum_{K=1}^{n_w} q_{out}^K, \qquad Q_t=\sum_{K=1}^{n_w} q_t^K \tag{6}$$

Equation (3) can now be written as:

$$\pi r_w^2 h_w \frac{\partial C_w}{\partial t}=Q_{in}C_{in}+\sum_K\left(q_t^K\left(C_t^K-C_w\right)-q_{in}^K C_w\right) \tag{7}$$

where C_t^K are the concentrations in the transit flow rates q_t^K at the n_w connecting nodes.

A time finite difference approximation of equation (7) is used between time N and $N+1$ (time step Δt), together with classical time approximations for concentration terms (ω_w is a time weighting factor, usually set to 1):

$$C_w(t)\approx \omega_w C_w^{N+1}+(1-\omega_w)C_w^N \tag{8}$$

$$\frac{\partial C_w(t)}{\partial t}\approx\frac{C_w^{N+1}-C_w^N}{\Delta t} \tag{9}$$

$$h_w(t)\approx h_w^*=\omega_w h_w^{N+1}+(1-\omega_w)h_w^N \tag{10}$$

This gives the following expression for the concentration evolution in the injection well:

$$C_w^{N+1}=\frac{1}{R_w}\left(Q_{in}C_{in}+\sum_K q_t^K C_K^N+B_w C_w^N\right)$$

with: (11)

$$R_w=\frac{\pi r_w^2 h_w^*}{\Delta t}+\omega_w\sum_K\left(q_t^K+q_{in}^K\right), \qquad B_w=\frac{\pi r_w^2 h_w^*}{\Delta t}-(1-\omega_w)\sum_K\left(q_t^K+q_{in}^K\right)$$

Aquifer concentrations C_k are evaluated explicitly to avoid the dependency of computed concentrations in the aquifer at one well node on the concentrations at the other well nodes.

Representing the solute transport equation by a general operator $T(C)$ including all processes (advection, dispersion, etc.) except injection terms, the following expression can be used to describe the coding of the injection well in any three-dimensional simulator:

$$T(C)-\sum_{K=1}^{n_w}\left(q_{out}^K C_w-q_t^K C_t^K\right)=0 \tag{12}$$

The resulting equation system has the following general form:

$$[R_C]\cdot\{C\}^{N+1}=\{G_b\}-\sum_{K=1}^{n_w} q_t^K C_t^{K,N}+\sum_{K=1}^{n_w} q_{out}^K\left(\omega_w C_w^{N+1}+(1-\omega_w)C_w^N\right) \tag{13}$$

The discrete form of C_w, equation (11), is introduced in equation (13) and the resulting system is solved.

EXAMPLE

The test presented here shows the ability of the injection well concept to model practical field tracer tests. Numerical simulations were conducted with the finite element simulator SUFT3D (Carabin & Dassargues, 1999; Brouyère, 2000). It consists in modelling a radially converging tracer test. The aquifer has a thickness of 8 m, saturated conductivity of 5.0×10^{-2} m s^{-1}, effective porosity of 0.05, longitudinal dispersivity of 2 m and transverse dispersivity of 0.5 m. The initial total heads are uniform at 10 m (aquifer fully saturated). A flow rate of 50 m^3 h^{-1} is pumped out of the well. The injection well is located 20 m away from the pumping well, and a sampling well is located mid-way (10 m) between them. Pumping well, injection well and sampling well radii are 10 cm and 2 cm and 5 cm, respectively. Distortion coefficients are 0.5 for the sampling well and 2.0 for the injection well. A unit mass of tracer diluted in a volume V_{inj} = 0.1 m^3 is injected in the well during a 2 hour period, T_{inj}. A water flush is conducted with a volume V_{fl} = 0.2 m^3 over a period T_{fl} = 900 s.

Figure 2 shows that the new approach is able to reproduce actual differences between the evolution of concentrations in the "experimental" injection profile (C_{inj}, T_{inj}), in the injection well $C_w(t)$ and in the aquifer around $C(t)$. It also allows comparison of the computed and field measured injection (or sampling) well concentrations. Classical approaches only provide aquifer concentration evolutions. Back diffusion of the tracer in the well is visible. It is due to a well concentration decrease to a level lower than in the surrounding aquifer. After the flush, the higher concentration in the transit flow rate boosts the well tracer concentrations. Such back-diffusion effects have been observed on field results conducted during this research. Due to the long duration injection, the concentration in the well reaches an equilibrium (C_w = 7.82 ppm/inj.kg) lower than the injection concentration (C_{inj} = 10.0 ppm/inj.kg). The injection rate Q_{inj} is lower than the critical injection rate Q_{cr} and a transit flow rate Q_t dilutes the concentrations in the well. As in point dilution methods, the measured degree of tracer dilution in the injection well can be used to evaluate local aquifer water fluxes.

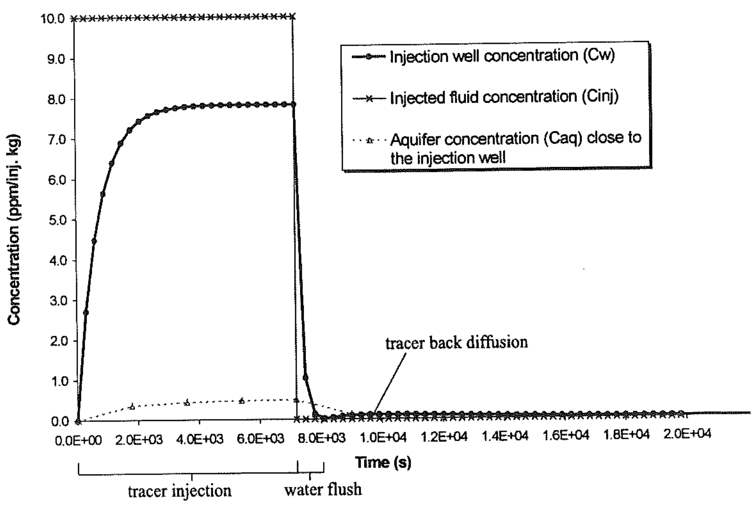

Fig. 2 Concentration evolution at the injection point.

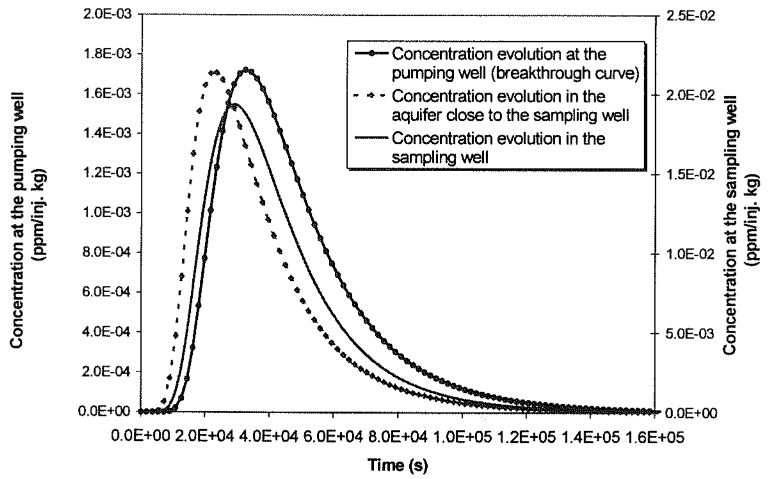

Fig. 3 Concentration evolution at the sampling and pumping wells.

Figure 3 shows the breakthrough curve at the pumping well. In this example, results obtained with the new approach or with a classical third-type boundary condition do not depart too much. Other tests (results not shown here) have demonstrated that the injection process can have a dramatic influence on the shape of the resulting breakthrough curve. In such cases, the use of a third-type boundary condition could lead to misinterpretation in terms of the aquifer transport parameters (i.e. overestimated dispersion and retardation). Figure 3 also shows concentration changes in the sampling well and in the surrounding aquifer. In the well, concentrations are delayed and attenuated. This effect, well known by experimenters (Robbins, 1989), can also lead to misinterpretation of tracer tests.

CONCLUSIONS

A new conceptual and mathematical approach is proposed to model the injection of a tracer in a well for field tracer tests. It can be easily implemented in any existing flow and transport numerical simulator. A simple test case has shown the improvement provided by applying the new concept to model complex field situations.

Further developments are envisaged. The concentration homogeneity in the injection well could be removed by using a full dual node formulation for the well nodes. The advantage would be that concentration variations along the well axis, which is often observed in point dilution methods, could be allowed for.

REFERENCES

Bidaux, P. & Tsang, C.-F. (1991) Fluid flow patterns around a well bore or an underground drift with complex skin effects. *Wat. Resour. Res.* **27**(11), 2993–3008.

Brouyère, S. & Rentier, C. (1997) About the influence of the injection mode on tracer test results. In: *Tracer Hydrology 97* (ed. by A. Kranjc), 11–17. A. A. Balkema, Rotterdam, The Netherlands.

Brouyère, S. (2000) Modelling of transport and retardation of solutes in variably saturated media. PhD Thesis, Faculty of Applied Sciences, University of Liège, Belgium.

Carabin, G. & Dassargues, A. (1999) Modeling groundwater with ocean and river interaction. *Wat. Resour. Res.* **35**(8), 2347–2358.

Drost, W., Klotz, D., Arnd, K., Heribert, M., Neumaier, F. & Rauert, W. (1968) Point dilution methods of investigating ground water flow by means of radioisotopes. *Wat. Resour. Res.* 4(1), 125–146.

Guvanasen, V. & Guvanasen, V. M. (1987) An approximate semianalytical solution for tracer injection tests in a confined aquifer with a radially converging flow field and a finite volume of tracer and chase fluid. *Wat. Resour. Res.* **23**(8), 1607–1619.

Klotz, M., Moser, H. & Trimborn, P. (1979) Single-borehole techniques. Present status and examples of recent applications. In: *Isotope Hydrology 1978*, 159–179. International Atomic Energy Agency, Vienna.

Moench, A. F. (1995) Convergent radial dispersion in a double-porosity aquifer with fracture skin: analytical solution and application to a field experiment in fracturated chalk. *Wat. Resour. Res.* **31** (8),1823–1835.

Novakowski, K. (1992) An evaluation of boundary conditions for one-dimensional solute transport, 1. Mathematical development. *Wat. Resour. Res.* **28**(9), 2399–2410.

Robbins, G. A. (1989) Influence of using purged and partially penetrating monitoring wells on contaminant detection, mapping and modeling. *Groundwater* **27**(2), 155–162.

Sudicky, E. A., Unger, A. J. A. & Lacombe, S. (1995) A non iterative technique for the direct implementation of well-bore boundary conditions in three-dimensional heterogeneous formations. *Wat. Resour. Res.* **22**(13), 411–415.