POLISH ACADEMY OF SCIENCES
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# MODELLING CONCEPTS AND DECISION SUPPORT IN ENVIRONMENTTAL SYSTEMS

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The purpose of the present publication is to popularize information tools and applications of informatics in environmental engineering and environment protection that have been investigated and developed in Poland and Germany for the last few years. The papers published in this book were presented during the workshop organized by the Leibniz-Institute of Freshwater Ecology and Inland Fisheries in Berlin in February 2006. The problems described in the papers concern the mathematical modeling, development and application of computer aided decision making systems in such environmental areas as groundwater and soils, rivers and lakes, water management and regional pollution. The editors of the book hope that it will support the closer research cooperation between Poland and Germany and when this intend succeeds then also next publications of the similar kind will be published.

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# CHAPTER 1

# Groundwater / Soil

# ASSESSING DYNAMICS OF INFILTRATION OF RIVER WATER TO WELL VIA AN EMPIRICAL MODEL

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***Abstract:*** *When operating an infiltration well supplied by river water a problem with high accidental pollution of the river water sometimes occurs. In this paper a possibility of developing of a simple model to help in managing such situation is investigated. The model includes a time delay and some dynamics. To estimate the model parameters some identificability problems have to be solved. The model is then validated using independent data in changed conditions, among which much smaller pumping ratio was found to be most important. Good prediction has been obtained, although a problem with finding an appropriate time delay has been spotted.*

**Keywords**: infiltration well, pollution, emergency management, modeling, system identification

## 1. Introduction

Infiltration wells located in river valleys are often exploited as a competitive alternative to direct pumping of water from rivers for municipal use. When operating the wells, an important, though perhaps not so frequent, problem is to manage emergency cases when, e.g. due to an accident, the river water carries harmful pollutants. A question then is whether to stop pumping the water from the wells and, if the answer is positive, when and for how long. To answer these questions knowledge of dynamics of infiltration of water from the river to the well is important. For this, detailed partial differential modeling of the water flow through the soil could be performed. This kind of modeling is usually a difficult task in the case of infiltration well, see e. g. modeling in some different cases: Chen (2003), Franzetti & Guadagnini (1996), Mironenko & Pachepsky (1998). Moreover, the model obtained in this way is unnecessary detailed for the practical use.

The problem considered in this paper is to investigate a possibility to develop a simple lumped parameter model to assess this dynamics. This is done using statistical methods of parameter estimation and system identification.

To use statistical methods some measurements are needed. Usually a tracer is applied for an appropriate experimentation in such cases as the one described here. To simplify the cost, we used as a tracer the common salt which is present in quite high concentrations in some Polish rivers. This choice of the tracer, albeit convenient for cheap and quick measurements, caused some problems described in the sequel.

The problem presented has been earlier partly described in the Polish literature, Nahorski at al. (1991), Lomotowski (1994), Nahorski & Lomotowski (1994). In this paper new results are included. They are concerned with identifiability analysis and presentation of the explicit formulae for calculating physical parameters of the continuous time model from the parameters of an auxiliary discrete time model, as well as with validation of the model using independent data.

## 2. A physical parameter model

The infiltration well considered, see Fig. 1, is located in the river bed. Its diameter is 11 m and the depth 40 m. The water is collected by 15 drains with diameter 0.3 m and the lengths between 85.5 m and 100 m lying at the depth 7 m from the river bed, see Fig. 2. The river bed aquifer is built from the Quaternary sand, with thickness of at least 20 m.

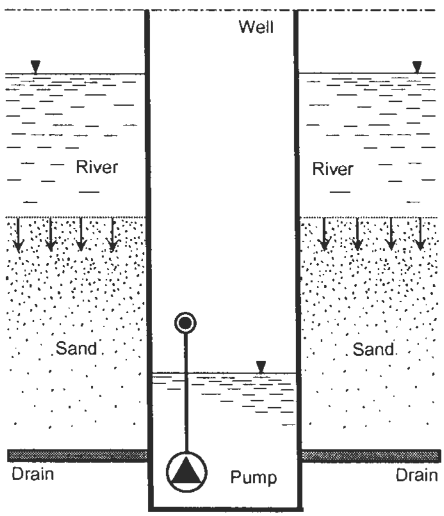


**Figure 1.** An infiltration well in the river bed.

When the pumping rate from the well is high, the vertical flow of water dominates in the area above the drains. Neglecting the horizontal flow, the movement of the salt dissolved in water, and more precisely the chlorine anions $Cl^-$, can be described by the equation

$$\frac{\partial c(z,t)}{\partial t} = D\frac{\partial^2 c(z,t)}{\partial z^2} - v\frac{\partial c(z,t)}{\partial z}$$

where $c(z, t)$ is the concentration of the anions $Cl^-$ at the depth $z$ in the time $t$, $v$ is the velocity of the water flow, and $D$ is the dispersion coefficient. If the velocity $v$ is high, the component connected with dispersion can be neglected. Then the movement of the salt can be approximated by the plug flow, in which the salt travels with water from the river to the drain through some time $t_d$, without any dispersing. Assuming now perfect mixing of water in the well, the partial differential model can be approximate by an ordinary differential one

$$\frac{dM(t)}{dt} = Q_{in}(t) - Q_{out}(t)$$

where $M(t) = V(t)c(t)$ is the mass of the $Cl^-$ anions in the well, being the product of the water volume in the well $V(t)$ and the concentration of the $Cl^-$ anions in the well water $c(t)$; $Q_{in}(t) = q_{in}(t)c_r(t - t_d)$ is the inflow of the $Cl^-$ anions to the well in the unit time, being the product of the inflow of water $q_{in}(t)$ and the concentration of the $Cl^-$ anions $c_r(t - t_d)$ in the river delayed by the travel time $t_d$; $Q_{out}(t) = q_p(t)c(t)$ is the outflow of the $Cl^-$ anions from the well in the unit time, being tha product of the pumping rate $q_p(t)$ and the concentration $c(t)$.

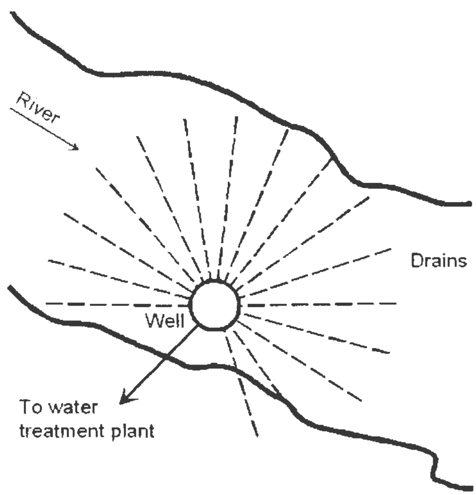


**Figure 2.** A schematic location of the well in the river.

We further assume that the water volume in the well does not change

$$\frac{dV(t)}{dt} = q_{in}(t) - q_p(t) = 0$$

that is, that $V(t) = V = \text{constant}$ and $q_{in}(t) = q_{out}(t) = q(t)$. Thus, the concentration of the $Cl^-$ anions in the well evolves according to the equation

$$V\frac{dc(t)}{dt} = q(t)\left[c_r(t-t_d) - c(t)\right] \tag{1}$$

This equation can be further simplified by change of variables, as proposed by Niemi (1988), see also Bogdan at al. (2000). This method is presented in the Appendix.

## 3. Discrete time model approximation

The data were measured in discrete times. We denote the time instants when the measurements were taken by $t_0, t_1, t_2, \ldots, t_N$.

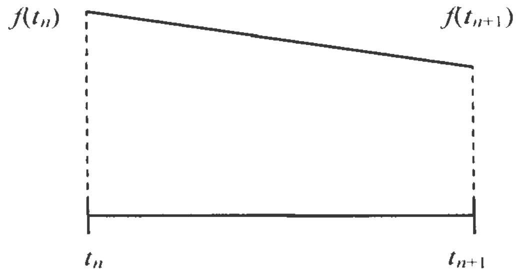


**Figure 3.** Trapezoidal rule of integration

The solution of (1) at $t = t_{n+1}$, $n = 0, 1, \ldots, N-1$, has the form

$$c(t_{n+1}) = c(t_0)a(t_0, t_{n+1}) + \frac{1}{V}\int_{t_0}^{t_{n+1}} a(\tau, t_{n+1})q(\tau)c_r(\tau - t_d)d\tau$$

where

$$a(\tau, t_{n+1}) = \exp\left[-\frac{1}{V}\int_{\tau}^{t_{n+1}} q(\varsigma)d\varsigma\right]$$

The above equation can be transformed as follows

$$c(t_{n+1}) =$$

$$= a(t_n, t_{n+1})\left\{c(t_0)a(t_0, t_n) + \frac{1}{V}\int_{t_0}^{t_n} a(\tau, t_n)q(\tau)c_r(\tau - t_d)d\tau\right\} + \frac{1}{V}\int_{t_n}^{t_{n+1}} a(\tau, t_{n+1})q(\tau)c_r(\tau - t_d)d\tau =$$

$$= a(t_n, t_{n+1})c(t_n) + \frac{1}{V}\int_{t_n}^{t_{n+1}} a(\tau, t_{n+1})q(\tau)c_r(\tau - t_d)d\tau \tag{2}$$

This equation requires knowledge of $q(t)$ within the period $[t_n, t_{n+1}]$, and $c_r(t)$ within the period $[t_n - t_d, t_{n+1} - t_d]$. As the measurements are taken only in discrete time, we use the trapezoidal rule of integration, see Fig. 3. For a generic function $f(\tau)$ it has the form

$$\int_{t_n}^{t_{n+1}} f(\tau)d\tau = \frac{1}{2}(t_{n+1} - t_n)[f(t_{n+1}) - f(t_n)]$$

For our integral in (2) we have

$$f(t_{n+1}) = q(t_{n+1})c_r(t_{n+1} - t_d) \qquad f(t_n) = a(t_n, t_{n+1})q(t_n)c_r(t_n - t_d)$$

As the values $c_r(t_{n+1} - t_d)$ and $c_r(t_n - t_d)$ need not be the measured ones, they have to be expressed by the measured values. For this we use a linear approximations explained in Fig. 4. The value $c_r(t_n - t_d)$ is approximated by a linear combination of measured values $c_r(t_{n-k-1})$ and $c_r(t_{n-k})$, with an appropriately chosen $k$, according to the following formula

$$c_r(t_n - t_d) \approx \frac{t_{n-k} - (t_n - t_d)}{t_{n-k} - t_{n-k-1}} c_r(t_{n-k}) + \left(1 - \frac{t_{n-k} - (t_n - t_d)}{t_{n-k} - t_{n-k-1}}\right) c_r(t_{n-k-1})$$

and similarly for $c_r(t_{n+1} - t_d)$

$$c_r(t_{n+1} - t_d) \approx \frac{t_{n-k+1} - (t_{n+1} - t_d)}{t_{n-k+1} - t_{n\;k}} c_r(t_{n-k+1}) + \left(1 - \frac{t_{n-k+1} - (t_{n+1} - t_d)}{t_{n-k+1} - t_{n-k}}\right) c_r(t_{n-k})$$

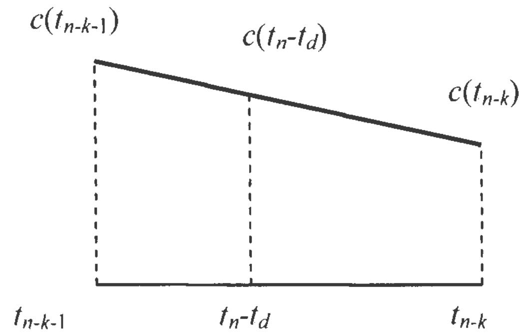


**Figure 4.** Linear approximation of delayed concentrations.

In the case considered the sampling interval was constant. We denote $t_{n+1} - t_n = \Delta$. Moreover, we assume that the flow is constant, i. e. $q(t) = q$ = constant. Then, also the value $a(t_n, t_{n+1})$ depends only on the difference $t_{n+1} - t_n$

$$a(t_n, t_{n+1}) = \exp(-q\Delta / V) = a$$

Let us recapitulate the assumptions made:

1. The vertical flow predominates above the drains.
2. The dispersion of the tracer can be neglected.
3. The pumping rate is equal to the inflow of the infiltrated water to the well.
4. The sampling interval is constant and known.

With these assumptions and the earlier introduced notation we finally have

$$c(t_{n+1}) = ac(t_n) + \frac{q\Delta}{2V}\left[(1-\frac{[t_d]}{\Delta})c_r(t_{n-k+1}) + \frac{[t_d]}{\Delta}c_r(t_{n-k}) + \right.$$

$$\left. + a\left((1-\frac{[t_d]}{\Delta})c_r(t_{n-k}) + \frac{[t_d]}{\Delta}c_r(t_{n-k-1})\right)\right] \tag{3}$$

where

$$[t_d] = t_{n-k} - (t_n - t_d).$$

For $k = 0$ it holds $[t_d] = t_d$. With the above approximations, the equation (3) takes a recursive form

$$c(t_{n+1}) = ac(t_n) + b_{k-1}c_r(t_{n-k+1}) + b_k c_r(t_{n-k}) + b_{k+1}c_r(t_{n-k-1}) \tag{4}$$

with the coefficients depending on physical parameters

$$a = \exp\left(-\frac{q\Delta}{V}\right) \qquad b_{k-1} = \frac{q\Delta}{2V}\left(1-\frac{[t_d]}{\Delta}\right)$$

$$b_k = \frac{q\Delta}{2V}\left[a\left(1-\frac{[t_d]}{\Delta}\right) + \frac{[t_d]}{\Delta}\right] \qquad b_{k+1} = \frac{q\Delta}{2V}\frac{a[t_d]}{\Delta} \tag{5}$$

Knowing the physical parameters $q$, $\Delta$, $V$ and $t_d$, it is possible to calculate the coefficients of the model (4).

However, we will be more interested in an inverse problem, which is calculation of $V$ and $t_d$, and possibly $q$[1], from the estimates $\hat{a}$, $\hat{b}_{k-1}$, $\hat{b}_k$, $\hat{b}_{k+1}$ computed from measurements. There are 2 or 3 unknown variables and 4 equations in (5). However, it can be noticed that $b_{k-1}$, $b_k$ and $b_{k+1}$ are linearly dependent, as it holds

$$ab_k = a^2 b_{k-1} + b_{k+1} \tag{6}$$

Thus, knowing $a$ and two of the three above coefficients the third can be found from the above relation. Also, one more dependence can be found

[1] Notice that $\Delta$ is known and $q$ may be also often known.

$$b_{k+1} + ab_{k-1} + 0.5a \ln a = 0 \tag{7}$$

Thus, there are only two independent equations among four in (5). As the parameters $q$ and $V$ are always present as the ratio $q/V$, then actually also only two values, $q/V$ and $t_d$, be calculated. Taking equations for $a$ and $b_{k-1}$ as the two independent ones, the following formulae can be derived

$$\frac{q}{V} = -\frac{1}{\Delta}\ln a \qquad t_d = \Delta\left(1 + 2\frac{b_{k-1}}{\ln a} + k\right) \tag{8}$$

The dependencies between parameters in equation (4) cause problems in estimation. Particularly (6) introduces the linear dependence, which results in bad numerical conditioning of matrices that are inverted in estimation algorithms.

## 4. Parameter and structure estimation

The data from measurements consisted of $Cl^-$ anions concentrations both in the river water and the well water, see Fig. 5. There were altogether 92 pairs of measurements taken once a day at 10 o'clock from March the 6th to June the 5th, 1989. Thus, the sampling interval was $\Delta$ = 1 day (24 h). The nominal pumping rate was $q$ = 300 000 m$^3$/d, but the actual pumping rate varied around this value, see Fig. 6.

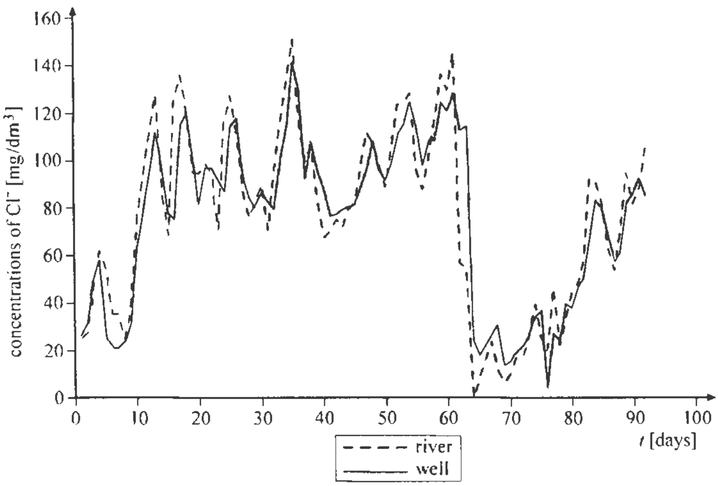


**Figure 5.** Observed concentrations of $Cl^-$ in the river and in the well.

The parameters in the model (4) were estimated using the least squares method. Other methods, which admit for correlated errors, has been also tried, but correlation coefficients were found statistically insignificant. Parameter estimates, with $k$ = 0, are shown in Table 1, model no. 4. It is noticeable that the estimates of the standard deviation of parameter estimates are quite big, particularly for the estimate $\hat{b}_2$, where it is bigger that the parameter estimate itself. Although no formal test is presented here, the estimate $\hat{b}_2$ is insignificant. This does not happen for the simpler models (nos. 1-3).

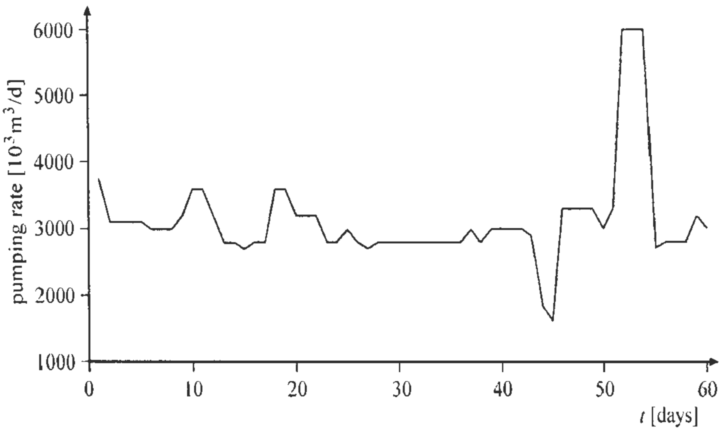


**Figure 6.** Real pumping rate during the experiment.

To help in choice of the best model some structure determination criteria, see e. g. Gustafsson & Hjalmarson (1995), were calculated. Two first criteria depicted in Table 2 take the smallest values for model no. 2. According to them the model no. 2 should be chosen as the best. This actually corresponds to the model (4) with dropped last term $b_{k+1}c(t_{n-k-1})$. This may be due to the linear dependence (6). The last criterion, BIC, suggest even to accept model no. 1, which may be caused by both dependencies (6) and (7).

**Table 1.** Results of estimation models with different structures. Values at parentheses are estimates of the standard deviations.

| Model no. | $\hat{a}$ $(\pm\hat{\sigma}_{\hat{a}})$ | $\hat{b}_0$ $(\pm\hat{\sigma}_{\hat{b}_0})$ | $\hat{b}_1$ $(\pm\hat{\sigma}_{\hat{b}_1})$ | $\hat{b}_2$ $(\pm\hat{\sigma}_{\hat{b}_2})$ |
|---|---|---|---|---|
| 1 | 0.450 (±0.041) | 0.526 (±0.038) | | |
| 2 | 0.327 (±0.067) | 0.457 (±0.048) | 0.184 (±0.082) | |
| 3 | 0.260 (±0.094) | | 0.683 (±0.089) | |
| 4 | 0.265 (±0.106) | 0.456 (±0.049) | 0.183 (±0.090) | 0.060 (±0.085) |

**Table 2.** Results of choice of structure criteria. The model with the smallest criterion value should be chosen.

| Model no. | Loss function | AIC | FPE | BIC |
|---|---|---|---|---|
| 1 | 9.60 | 681 | 96 | 2.36 |
| 2 | 9.34 | 678 | 93 | 2.38 |
| 3 | 13.16 | 739 | 181 | 2.68 |
| 4 | 9.30 | 681 | 96 | 2.43 |

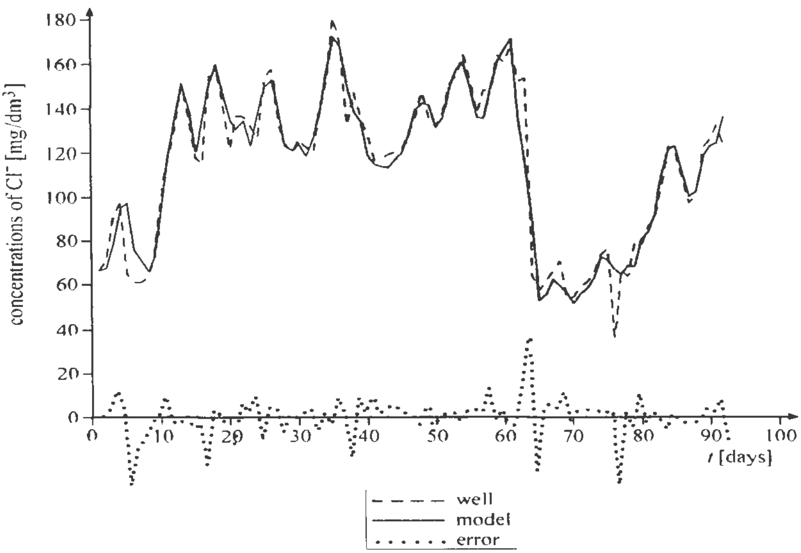


**Figure 7.** Fit of the model to the observed concentrations in the well.

Finally the best estimated model is

$$c(t_{n+1}) = 0.327c(t_n) + 0.457c_r(t_{n+1}) + 0.184c_r(t_n) \tag{9}$$

or

$$c(t_{n+1}) = 0.450c(t_n) + 0.526c_r(t_{n+1}) \tag{10}$$

The fit to the data of the model (9) is shown in Fig. 7. Inserting the estimates $\hat{a}$ and $\hat{b}_0$ to equations (8) with $q = 300\ 000\ \mathrm{m^3/d}$, the following estimates can be calculated

$$\hat{V} = 270\ 000\ \mathrm{m^3} \qquad \hat{t}_d = 4.5\ \mathrm{h} \tag{11}$$

for the model (9), and

$$\hat{V} = 375\ 000\ \mathrm{m^3} \qquad \hat{t}_d = -7.6\ \mathrm{h} \tag{12}$$

for the model (10). The geometrical volume of the well together with the drains is around 1000 $m^3$. Thus, $\hat{V}$ are rather estimates of the volume of the attraction cone. The negative value of the delay for the model (10) makes it useless and will not be discussed in the sequel.

Inserting further the rounded off estimates $\hat{V}$ and $\hat{t}_d$ from (11) to the equations (5), the following estimated full equation (4) can be obtained

$$c(t_{n+1}) = 0.329c(t_n) + 0.451c_r(t_{n+1}) + 0.253\,c_r(t_n) + 0.034c_r(t_{n-1})$$

## 5. Cross-validation of the model using independent data

The model has been checked using independent data gathered approximately two years later, from September 27th to October 4th, 1991. The sampling interval was chosen as $\Delta$ = 3h. The nominal pumping rate was at that time $q$ = 90 000 $m^3$/d. The conditions in both presented here experiments are compared in Table 3. With these new values and previous estimates $\hat{V}$ and $\hat{t}_d$ the new estimates of parameters in equation (4) could be calculated. However, a question is whether the volume $V$ and the time delay $t_d$ did not change with new conditions, and particularly with much smaller pumping rate $q$.

**Table 3.** Comparison of conditions for two experiments.

| | New experiment | Previous experiment |
|---|---|---|
| Number of samples | $N = 60$ | $N = 92$ |
| Sampling interval | $\Delta = 3$ h | $\Delta = 24$ h |
| Pumping rate | $q$ = 90 000 m3/d | $q$ = 270 000 m3/d |
| Season | early autumn | late spring |

Let us look at the data from the new experiments, depicted at in Fig. 8. An astonishing phenomenon is that while the concentration of $Cl^-$ in the river changes slowly, the concentration in the well varies quite rapidly. This is completely contrary to the intuition.

Let us, however, concentrate only on the measurements taken at 10 o'clock, marked with dots at Fig. 9, and connected by a piecewise linear function. This function does not vary too much. Moreover, it resembles a delayed concentration curve in the river. Closer examinations revealed that the effect of quick variations of concentrations in the well was connected with a big power and electricity plant located upstream of the well. The plant runs off salt water to the river by a pipe with an outlet under the river surface. The salt water does not mix so quickly with river water but flows at the bottom of the river. It infiltrates to the well and influences concentrations there.

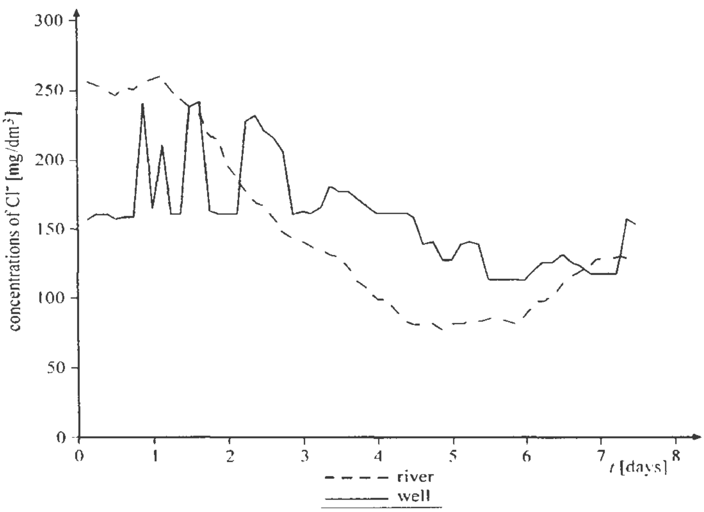


**Figure 8.** Observed concentrations of $Cl^-$ in the river and in the well for the new data.

Measurements of concentrations in the river were, however, taken from the surface water, not contaminated by the salt water from the plant. The run off from the plant was cyclical and around 10 o'clock stopped or was minimal. Thus, it was not found in the measurements taken once a day in the experiment.

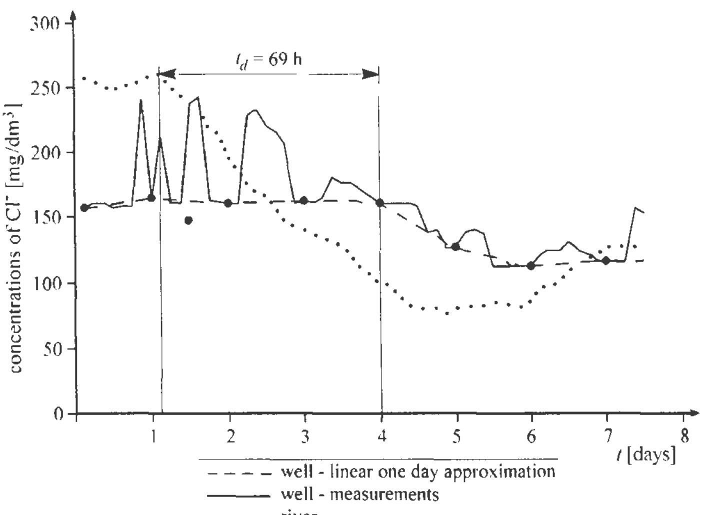


**Figure 9.** Piecewise linear approximation of one-day measurements and estimation of delay.

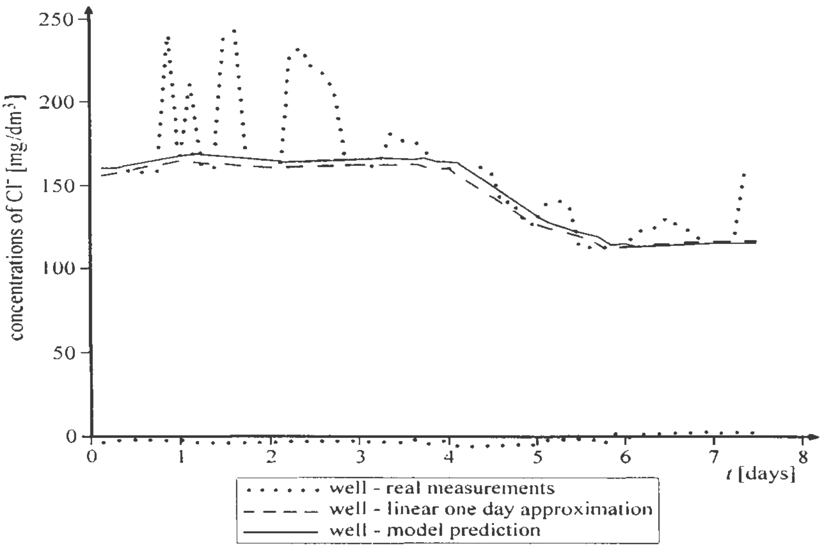


**Figure 10.** Approximated measured concentrations in the well and the model predictions.

Knowing this and cutting off this additional concentration, we can imagine that the evolution of concentrations in the well follows that of the river with a delay, which can be at this case estimated directly from the diagram, see Fig. 9, as $\hat{t}_d = 69\text{h}$ , or $k$ = 23. Inserting this value, together with the previous estimate of the volume, $\hat{V} = 270000\text{m}^3$, to the equations (5), the following model is obtained

$$c(t_{n+1}) = 0.959c(t_n) + 0.021[c_r(t_{n-22}) + 0.959c_r(t_{n-23})]$$

This model predicts quite well the piecewise linear function connecting the 10 o'clock once-a-day measurements, although there is a small bias, which can be due to errors in estimates of $V$ or $t_d$, see Fig. 9.

## 6. Conclusions

An important finding from the investigations presented is that a simple linear lumped parameter model can give good fit to the measurements from a real well, and a good prediction, provided a good estimate of the pure delay is given. The delay seems, however, to depend strongly on the pumping rate from the well. This relation is unknown and its lack is a main obstacle in application of the model. Also dependence of the volume $V$ on the pumping rate is unknown, albeit it seems to be of a secondary importance.

Some improvements of the algorithm described in the paper can be made, see the Appendix. The improvement proposed is connected with extension of the model to a variable pumping rate, which must be, however, measured. Another improvement could be connected with development of an algorithm, which takes into account the problem of dependence of parameters.

## Appendix. Variable flow case

Let us introduce a new variable, the integrated water flow from time $t_0$ to $t$

$$\xi(t) = \int_{t_0}^{t} q(\tau) d\tau$$

As $q(\tau) > 0$, then there exists the inverse function $t = t(\xi)$. We denote $c(\xi) = c(t(\xi))$. Then

$$\frac{dc(t)}{dt} = \frac{dc(\xi)}{d\xi}\frac{d\xi}{dt} = \frac{dc(\xi)}{d\xi} q(t)$$

and therefore

$$V\frac{dc(\xi)}{d\xi} q(t) = q(t)\left[c_r(\xi - \xi_d) - c(\xi)\right]$$

where $\xi_d = \xi(t_d)$. After reduction of $q(t)$ in both sides we get an equation with a constant parameter

$$V\frac{dc(\xi)}{d\xi} = c_r(\xi - \delta) - c(\xi)$$

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## MODELLING CONCEPTS AND DECISION SUPPORT IN ENYIRONMENTAL SYSTEMs

This book presents the papers that describe the most interesting results of the research that have been obtained during the last few years in the area of environmental engineering and environment protection at the Systems Research Institute of the Polish Academy of Sciences in Warsaw and the Leibniz-Institute of Freshwater Ecology and Inland Fisheries in Berlin (IGB). The papers were presented during the First Joint Workshop organized at the IGB in February 2006. They deal with mathematical modeling, development and application of computer aided decision making systems in the areas of the environmental engineering concerning groundwater and soil, rivers and lakes, water management and regional pollution.

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