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Risk assessment of well contamination using a regional stochastic modelling approach

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ABSTRACT : This paper presents a stochastic risk analysis approach for contamination of water supply wells in agriculturally dominated catchment areas, using a stochastic approach, where a numerical one-dimensional pesticide transport model has been coupled with a numerical three-dimensional groundwater flow- and transport model. The risk analysis is based on Monte-Carlo simulations with multiple realizations of the entire parameter set at a scale of individual agricultural fields. For the generation of the parameter set in the saturated zone the turning band method was used according to the lognormal pdf.

Based on a set of soil and aquifer data from literature, the importance of different soil parameter distributions and different agricultural area sizes, were analysed with respect to the variability of the concentration breakthrough curves as observed at an assumed groundwater supply well. Using the coupled stochastic modelling approach the risk of exceeding a given concentration limit was investigated as a result of spatially variable soil and aquifer transport properties.

1. INTRODUCTION

Contamination by agricultural activities became a severe problem for groundwater quality in many regions used for water supply **[Leistra, Boesten 1989]**,**[Cohen 1991]**. With respect to pesticides the European Community (EC) therefore decided 1980 to introduce regulations concerning the concentration of pesticides in groundwater **[EG 1980]**. According to this regulation, in the FRG the concentrations were limited to 0.1 $\mu g/l$ for a single active substance and to 0.5 $\mu g/l$ for the sum of all substances including metabolites **[BMJFG 1986]**.

Considering the complexity of the processes involved in the fate and transport of pesticides through the unsaturated and saturated zone, e.g. the transformation into metabolites and sorption, **[Saltzman,Mingelgrin 1984]**, and the limited hard data usually availabel for regional-scale modelling, it becomes obvious that parameter uncertainty has to be considered when groundwater quality predictions are seriously attempted.

An objective approach is to use geostatistical-stochastic methods which takes into account the variability of the measured parameters including their spatial correlation **[Matheron 1971]**. This approach is in general preferable to the commonly used sensitivity analysis, because it directly leads to a quantitative representation of data density, data variability and data distribution.

Various deterministic modelling tools were used in conjunction with statistical and geostatistical parameter generators following a Monte-Carlo simulation. The physical principles of the deterministic modelling tools are presented in chapter 2, the regional modelling and the stochastic approach are presented in chapter 3 resp. chapter 4. Chapter 5 deals with the setup of the numerical experiment and chapter 6 contain the results and their discussion.

2. PHYSICAL PRINCIPLES

2.1 Water flow calculation

Water flow calculation in the unsaturated zone is based on Richard's equation (1).

$$\frac{\partial h}{\partial t}\frac{\partial \Theta}{\partial h} = \frac{\partial}{\partial z}\left[K(\Theta)\frac{\partial h}{\partial z}\right] - U(z,t) \qquad (1)$$

It states a relation beween the water content Θ and the piezometric head h. Root water uptake, precipation and evaporation are introduced by the sink/source term U. The relative hydraulic conductivity $K(\Theta)$ is calculated according to **[Campbell 1974]**.

Water flow in the saturated zone is calculated by the general three-dimensional differential equation (2), where K_s represents the tensor of the saturated hydraulic conductivity, and S_y denotes the specific yield. Groundwater recharge is represented by the source term N and discharge is represented by the sink term I.

$$S_y\frac{\partial h}{\partial t} = -\nabla\left(\underline{\underline{K}}_s\nabla h\right) + N - I \qquad (2)$$

The differential equations (1) and (2) are coupled. The conditions are such that the water flux at the bottom of the unsaturated zone equals the water flux at the top of the saturated zone and the capillary pressure at the bottom of the unsaturated zone model is determined by the vertical distance to the piezometric surface.

2.2 Transport calculation

Transport in the unsaturated zone is calculated using a one-dimensional advection-dispersion equation (Eq. 3).

$$\frac{\partial C\left(\Theta + \rho_b K_d\right)}{\partial t} = \frac{\partial}{\partial z}\left(\Theta D(\Theta, v)\frac{\partial C}{\partial z} - vC\right) + I \qquad (3)$$

In the saturated zone a three dimensional equation is used (Eq. 4).

$$\frac{\partial C\left(1 + \rho_b K_d\right)}{\partial t} = \nabla\left(\underline{\underline{D}}\nabla C - vC\right) + I \qquad (4)$$

In both equations K_d denotes the sorption coefficient, D the dispersion coefficent, and v the pore-water velocity. The calculation of the sorption coefficient in the unsaturated zone model is done by Eq. 5,

$$K_d = f_{oc}\cdot K_{oc} \qquad (5)$$

where K_{oc} denotes the organic carbon distribution coefficient and f_{oc} the organic carbon content of the soil.

Natural decay of the pesticide is introduced in the models through the sink/source term I employing a first order approach (Eq. 6),

$$\frac{\partial C}{\partial t} = K_{\mathrm{Dec}}\cdot C \qquad (6)$$

where K_{dec} represents the decay rate constant of the specific pesticide. A parameter to characterize the decay is the time to reach 1/2 of the initial concentration the so called half-life time.

The differential equations (3) and (4) are coupled by the condition that the mass flux through the bottom of the unsaturated zone is the mass flux to the top of the saturated zone. Mass flux from the saturated zone to the unsaturated zone due to capillary movement is neglected.

The transport equation is solved numerically by a finite difference scheme for the unsaturated zone and the method of characteristics for the saturated zone.

3. REGIONAL MODELLING APPROACH

In order to cover the entire range of measurements of the transport parameters e.g. saturated hydraulic conductivity, unsaturated hydraulic conductivity, sorption coefficient and decay rate, the following approach was chosen. It was decided that the data from the unsaturated zone is representative at the scale of the saturated model cells (a few tens of meters). This means in practical terms that we do not attempt to model the variability of the unsaturated flow and transport below the level of individual agricultural fields. The small scale variability is believed to be irrelevant with respect to the concentration levels observed at catchment scale. Consequently, when considering the soil parameter input for the unsaturated zone model one has to bear in mind that the data should represent the average properties of an entire agricultural field, i.e. should come from mixed soil samples.

4. STOCHASTIC MODELLING CONCEPT

As mentioned in chapter 1, the parameter values for the models are not selected deterministically, but generated using a statistical approach. From literature it is known that the variability

Table 1: Model input for the unsaturated zone

DETERMINISTIC	STOCHASTIC
Profile depth, bulk density, C_{Org}, climate timeseries	K_s, K_{OC}, Half-Life

Table 2: Model input for the saturated zone

DETERMINISTIC	STOCHASTIC
hydraulic configuration, input area	$\underline{\underline{K}}$

Table 3: Variation of statistic parameters

	σ_{lnK}	L_D/λ	B_F/λ	A_{IN}/A_{CA}
MIN	0.219	100	2.5	0.03
MAX	0.967	20	17.7	0.17

Table 4: Coefficients of variation for output of unsaturated zone model

	CV_{IN}	CV_{OUT}
K_s	0.30	0.02 ... 0.36
K_{oc}	0.45	2.08 ... 2.29
Half-life	0.53	0.704 ... 1.59

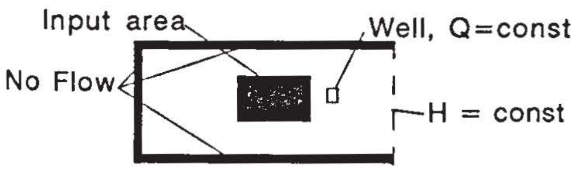

Figure 1: Hydraulic configuration for the saturated zone model

of the unsaturated hydraulic conductivity is very high, but the correlation length in the horizontal direction is much smaller than the average field size (tens of meters) (**[Ellsworth et. al. 1991]**, **[Parkes,Waters 1980]**, **[Russo,Bouton 1992]**, **[Wierenga et. al. 1991]**). Given the horizontal dimension of the saturated model cells, the single agricultural fields are therefore assumed to be spatially uncorrelated. Consequently the parameter distribution in the unsaturated zone in the horizontal direction was generated using a simple random number generator.

The generation of the 3-dimensional parameter distribution in the saturated zone had to include the spatial correlation between the individual model cells, since the correlation length in the saturated zone is typically much larger than the average model cell size, as shown by many field investigations, e.g. **[Hoeksema,Kitandis 1985]**, **[Sudicky 1986]** and **[Garabedian et.al. 1991]**. Assuming a lognormal probability distribution of the parameters and an exponential covariance structure, a Turning Bands Generator was used to generate the hydraulic conductivity in the saturated zone **[Tompson et.al 1989]**.

5. NUMERICAL EXPERIMENT

The numerical model used for the calculations is based on a combination of LEACHM **[Wagenet,Hutson 1987]**, MODFLOW **[McDonald, Harbaugh 1984]**, and a particle tracking code.

The model input for each zone is divided into a deterministic and a stochastic part. The parameters used in the simulation for the unsaturated and the saturated zone model are presented in Tab. 1, Tab. 2 and in Fig. 1 respectively. The data for the unsaturated zone stem from field measurements and are described in **[Harter,Teutsch 1990]**, **[Jury 1985]** and **[Jury et.al. 1987]**.

According to the modelling concept described in chapter 4 the statistical parameters of the random hydraulic conductivity field in the saturated zone were varied. The Variation is shown in table 3. The numerical experiment was designed to provide answers to the following questions:

1. What is the variation in pesticide mass flux at the interface between the unsaturated and saturated zone, given the soil parameter distribution shown in table 1?
2. What is the variation of the pesticide mass flux at the extracting water wells, downgradient of the agricultural area?

6. RESULTS AND DISCUSSION

6.1 Analysis of the variance in the unsaturated zone

Fig. 2 shows the ensemble of breakthrough

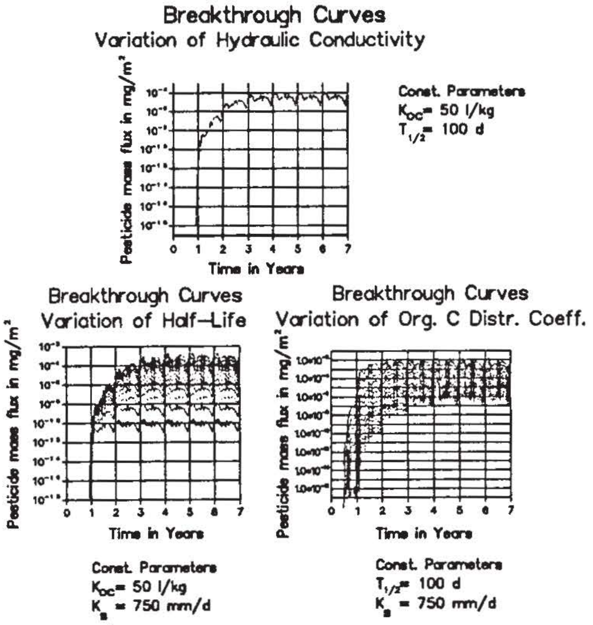

Figure 2: Breakthrough curves of Atrazine at the unsaturated/saturated interface for different parameter sets

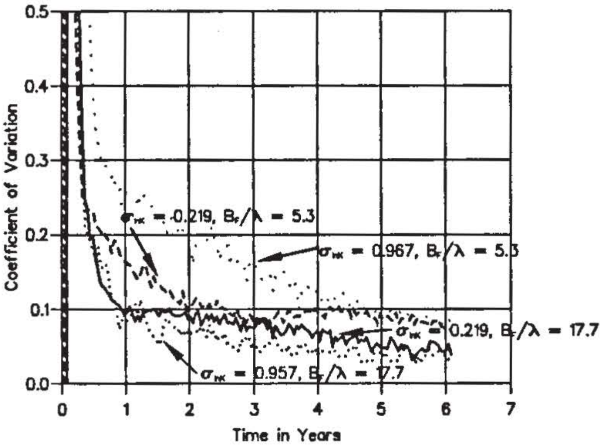

Figure 3: CV of BTCs for $A_{\mathrm{INPUT}}/A_{\mathrm{CATCH}} = 0.17$, λ and σ variable

curves (BTCs) as calculated by the unsaturated zone model. The coefficient of variation (CV), Eq. (7), is used to evaluate the BTCs, where μ denotes the average concentration at time t_i and σ is the standard deviation of the BTCs at time t_i.

$$CV_i = \left(\frac{\sigma}{\mu}\right)_i \tag{7}$$

The results of the simulation in the unsaturated zone are summarized in table 4. Based on the CV, the variation of the input parameters hydraulic conductivity, organic distribution coefficient and half-life is compared to the variation of the resulting BTCs at the unsaturated/saturated zone interface. It can be seen, that in the case of the variation of hydraulic conductivity, the resulting coefficient of variation of the BTCs is much lower than for the variation of the organic carbon distribution coefficient and half-life parameters. Obviously the sensitivity of the unsaturated zone model is smallest for the hydraulic conductivity parameter variation.

6.2 Results of the coupled model

As in the case for the BTCs at the unsaturated/saturated interface the CV of the BTCs at the extraction well is investigated.

The following observations seem important:

1. Fig. 3 shows clearly that the CV increases if the correlation length is increased.
2. The change in the variance of the hydraulic conductivity does not alter the asymptotic value of the CV but the temporal behaviour of the CV
3. Fig. 4 shows that the asymptotic value of the CV does not depend on the correlation length if the input area is small compared to the catchement area

6.3 Comparison with analytical solution

It can be shown that the CV can be described by

$$CV_{\mathrm{BTC}}(t) = \frac{1}{\sqrt{n_f(t)}} \cdot CV_{\mathrm{INPUT}} \tag{8}$$

CV_{INPUT} denotes the coefficient of variation of the mass input, CV_{BTC}, the coefficient of variation of the breakthrough curves and n_f represents the number of single fields which are located within the u catchement of the extraction well at time t. This equation can be transformed to

$$n_f(t) = \left(\frac{CV_{\mathrm{INPUT}}}{CV_{\mathrm{BTC}}(t)}\right)^2 \tag{9}$$

Eq. 9 can be interpreted as the cumultative probability density function (cdf) of traveltime of the fields. According to **[Dagan 1989]** this cdf can be expressed by:

$$G_T(\tau, A) = \int_A \frac{1}{2}\mathrm{erfc}\left\{\frac{L(\underline{x}) - U\tau}{\sqrt{2D_{ef}\tau}}\right\} dA \qquad (10)$$

if the average head gradient is constant and the particle position pdf is gaussian. In this equation $L(\underline{x})$ is the transport distance from the point $\underline{x} = (x_1, x_2)$ to the well and U is the average porewater velocity. D_{ef} denotes the effective dispersion coefficient. For small source areas the effective dispersion coefficient is given by **[Dagan 1991]** for non ergodic transport:

$$D_{eff}(t, l_1, l_2) = \frac{4}{l_1^2 l_2^2}\int_0^{l_1}\int_0^{l_2}\int_0^{t}(l_1 - b_1)(l_2 - b_2)[u_{11}(Ut', 0) - \frac{1}{2}u_{11}(Ut' + b_1, b_2) - \frac{1}{u_{11}}2(Ut' - b_1, b_2)]dt'\, db_2\, db_1$$

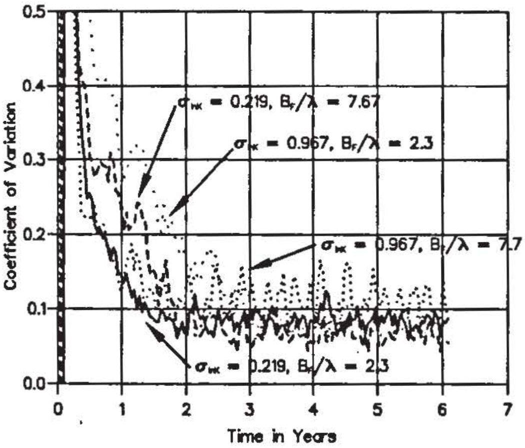

Figure 4: CV of BTCs for $A_{\text{INPUT}}/A_{\text{CATCH}}$ = 0.03, λ and σ variable

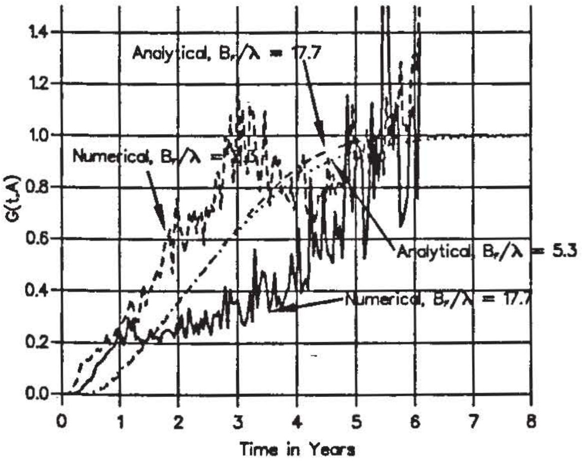

Figure 5: Numerical travel time cdf compared to analytical travel time cdf, $A_{\text{INPUT}}/A_{\text{CATCH}}$ = 0.17

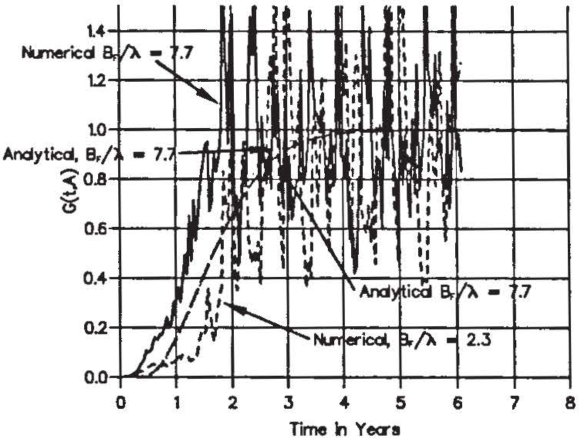

Figure 6: Numerical travel time cdf compared to analytical travel time cdf, $A_{\text{INPUT}}/A_{\text{CATCH}}$ = 0.03

l_1 and l_2 represent the input area dimensions, U is the average transport velocity and u_{11} is the two particle covariance.

Fig. 5 and Fig.6 show the cdf calculated by the coupled numerical model and the cdf according to **[Dagan 1989]** for different correlation lengths. It can be observed that only in the case of the small input area, the cdf of the coupled model can be represented in the average by the cdf according to **[Dagan 1989]**. This can be explained by the fact, that for the larger input area the assumption of the average constant gradient for the whole transport process no longer holds and therefore the calculation of the cdf has to be done still numerically.

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