

SIWAPRO DSS: A TOOL FOR COMPUTER AIDED FORECASTS OF LEACHATE CONCENTRATIONS

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KEYWORDS

Model, leachate concentration, unsaturated zone.

ABSTRACT

Leachate forecasts are claimed to evaluate the hazard to the groundwater caused by contaminations in the subsurface. It is advisable to employ a numerical model to simulate the complex nature of hydraulics and solute transport in the unsaturated zone. However many parameters are needed to formulate an appropriate simulation model. To minimize the efforts and the costs of exploration, knowledge of the main processes is necessary. Scenario and sensitivity analyses were done to evaluate the influence of each parameter on the results. The analyses showed, that there is no need for transient simulation if the solute is not degradable. On the contrary, if there are organic compounds, the solute concentration is very high subjected to time and also to degradation.

INTRODUCTION

Leachate forecasts are claimed to evaluate the hazard to the groundwater caused by contaminations in the subsurface. The source is described by a concentration either in the leachate or in the soil vs. time. The hazardous material is subjected to retardation and in some cases also to degradation or decay during its transport as solute through the unsaturated zone to the saturated or groundwater zone.

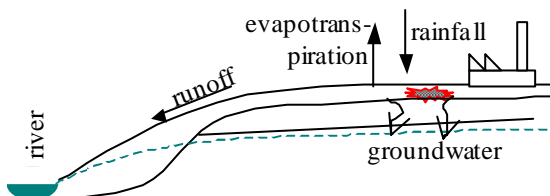


Figure 1: Illustration Figure

Because of the complex nature of soils and their transport properties it is recommended to use computer models for the leachate forecast. But quite a lot of parameters are needed to describe the properties of the source, of the transport through a heterogeneous unsaturated zone and also of the climatical boundary conditions and

the fluctuating groundwater table. The assessment of these parameters is expensive and prone to errors, the uncertainty of the values is very high.

Therefore we need to know, which parameters are really important to the result and need to be assessed most accurately and which parameters do not have such an influence on the calculated concentration in the leachate. In a first step, we took a real case for our scenario-/sensitivity analyses of boundary conditions and parameters. At the chosen site a chromium plating factory was established. The factory started at the end of the sixties and worked until the beginning of the nineties. A massive groundwater contamination with chromium and chromate was detected during the investigations in the nineties. The arising questions were

1. what will be the highest chromate concentration in the leachate
2. how long does it take until the max. concentration reaches the groundwater table
3. which chromium mass will enter the groundwater per year

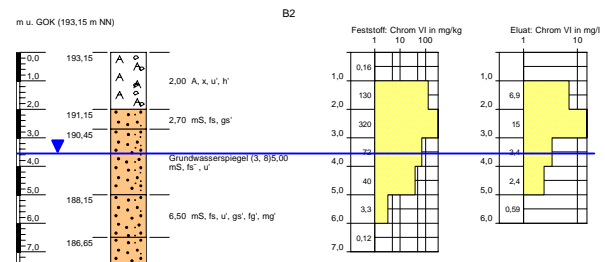


Figure 2: Soil and Concentration Profile at Location B2

MODELS

The scenario and sensitivity analysis were done using the computer program SiWaPro DSS. The name is the german synonym for Sickerwasserprognose (leachate forecast) Decision Support System. The program is based on the commonly used simulation code SWMS_2D (Šimunek et al. 1994).

Flow Model

The flow model describing unsaturated one dimensional vertical water flow in the unsaturated zone is given by RICHARD's-equation (1)

$$\frac{\partial}{\partial z} \left(k(\theta) \cdot \left(\frac{\partial h_p}{\partial z} + 1 \right) \right) = \frac{\partial \theta}{\partial t} - w_0 \quad (1a)$$

and

$$\frac{\partial \theta}{\partial t} = C(h_c) \cdot \frac{\partial h_p}{\partial t} \quad (1b)$$

where the independent variables are time t and spatial coordinate z . The dependent variables of equation (1) are the water pressure head $h_p = p_w / \rho_w \cdot g$ ($h_c = -h_p$) and the water content θ . w_0 is the sink/source term. The capillary capacity function $C(h_c)$ is the first derivative of the hysteretic soil water retention curve drawn in Figure 3. The unsaturated hydraulic conductivity $k(\theta)$ depends on the water content in the soil.

The hysteretic parametric model of soil water retention curve is given after van Genuchten (1980) and Luckner et al. (1989) by:

$$\theta = A + \frac{\phi - A - B}{\left[1 + (\alpha \cdot h_c)^n \right]^{\frac{1}{n}}} \quad (2)$$

The parameters of equation (2) are the porosity ϕ , the residual water content $\theta_{W,r}$, the residual air content $\theta_{A,r}$, the scaling factor α and the slope parameter n . Figure 3 shows a typical curve set for this hysteretic function, where

- | | | |
|---|-----|-------------------------|
| ① | PDC | Primary Drainage Curve |
| ② | SWC | Scanning Wetting Curve |
| ③ | SDC | Scanning Drainage Curve |
| ④ | MWC | Main Wetting Curve |
| ⑤ | MDC | Main Drainage Curve |

The function of unsaturated hydraulic conductivity was modeled by Mualem (1976) and Luckner et al. (1989) with

$$k(\theta) = k_0 \cdot \left(\frac{\bar{S}}{\bar{S}_0} \right)^\lambda \cdot \left[\frac{1 - \left(1 - \bar{S}^{\frac{1}{m}} \right)^m}{1 - \left(1 - \bar{S}_0^{\frac{1}{m}} \right)^m} \right]^2 \quad (3)$$

The parameters of equation (3) are the hydraulic conductivity $k_0(\theta_0)$ at a known degree of water mobility $\bar{S}_0 = (\theta_0 - \theta_{W,r}) / (\phi - \theta_{W,r})$, the parameter λ and the transformation parameter m . The function of unsaturated hydraulic conductivity is shown in Figure 4.

The parameters ϕ , k_0 and θ_0 must be estimated in advance using lab and/or field tests. The parameter λ in our model may range between $0 < \lambda < 1$, but it is kept fixed at $\lambda = 0.5$.

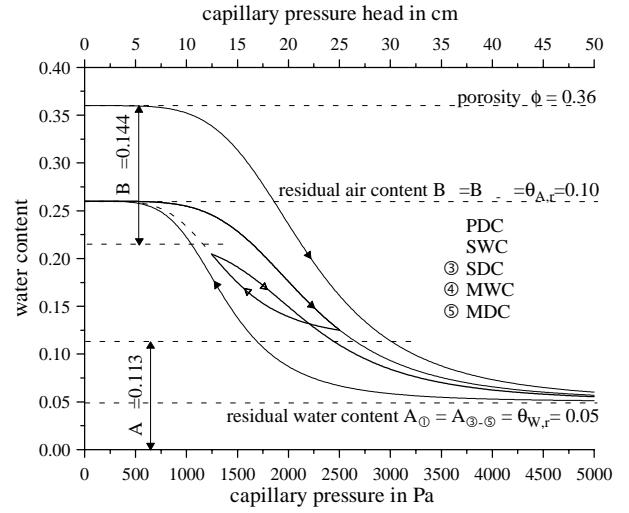


Figure 3: Hysteretic Soil Water Retention Curve

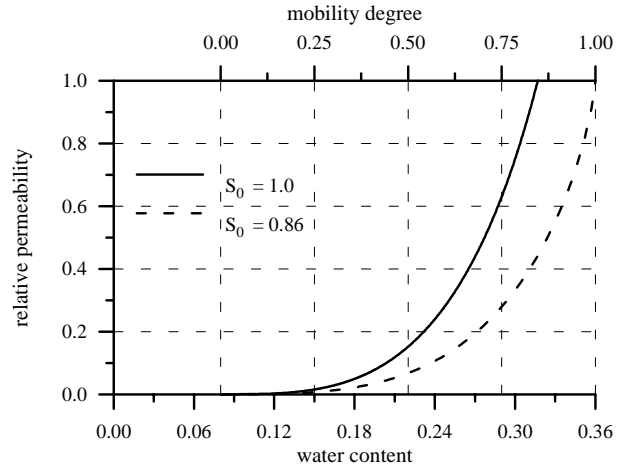


Figure 4: Relative Hydraulic Conductivity Function

Transport model

The well known convection-dispersion-equation (4) is used to describe the transport processes in the unsaturated zone.

$$\underbrace{\frac{\partial}{\partial r} \left(D \cdot \frac{\partial s_{fl,m}}{\partial r} \right)}_{\text{dispersion}} - \underbrace{\frac{\partial (u \cdot s_{fl,m})}{\partial r}}_{\text{convection}} = \underbrace{\frac{\partial s_m}{\partial t}}_{\text{mass storage changes}} + \underbrace{\mu_m \cdot s_m + \gamma_m \cdot \theta}_{\text{degradation terms}} - \underbrace{q_m}_{\text{sinks/sources}} \quad (4)$$

where is

r	m_R	spatial coordinate
t	s	time
θ	m^3 / m^3	water content
D	m^2 / s	dispersion coefficient ($D = \delta \cdot v $)
δ	m	dispersivity
s_m	kg / m^3	total specific mass ($s_m = s_{fl,m} + s_{s,m}$)

$s_{fl,m}$	kg / m_R^3	spezific mass in the liquid phase
$s_{s,m}$	kg / m_R^3	spezific mass in the solid phase
u	m_R / s	mean flux
γ_m	$\text{kg} / (\text{m}_{fl}^3 \cdot \text{s})$	0 order degradation coefficient
μ_m	s^{-1}	1. order degradation coefficient
q_m	$\text{kg} / (\text{m}_R^3 \cdot \text{s})$	sinks/sources

R,fl,B indexes the space, the liquid and and the soil

The convection term describes the solute transport with the water flux in the unsaturated zone. The dispersion term in equation (4) is the sum of the molecular diffusion and the hydrodynamic dispersion. Both processes are caused by concentrations gradient. The hydrodynamical dispersion is always bound to convection, but molecular diffusion is independent from it and may appear without any convection.

The dispersivity is an empirical parameter, it is a measure of heterogeneity of the soil and therefore depends on the scale. The reasons for dispersion are

- different velocities in the pore channels
- different pore sizes and therefore different velocities
- different flow times because of different flow paths
- transversal spreading of particles

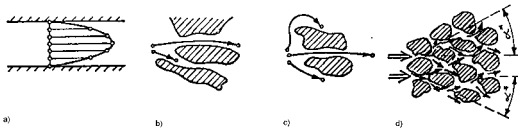


Figure 5: reasons for dispersivity in pore scale (figure taken from Luckner & Shestakov 1991)

Figure 6 shows an example for the results of dispersion in a column experiment. A short input (DIRAC impulse) was adapted on the upper boundary condition.

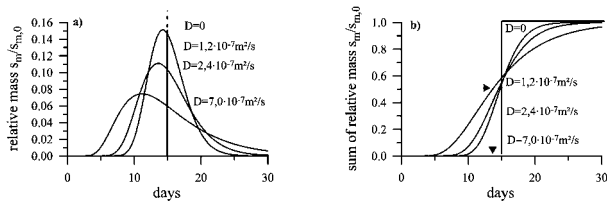


Figure 6: influence of dispersivity on breakthrough curves

The reason for retardation is sorption. The parameter describing the linear distribution function between the solute in the liquid and at the solid phase is the distribution or HENRY-coefficient K_D . The distribution and the retardation coefficient R are related to each other through equation (5). figure 7 shows the influence of retardation of the breakthrough curve at the bottom of a column experiment.

$$K_d = (R - 1) \cdot \frac{\theta}{\rho_b} \quad (5)$$

where ρ_b is the bulk density of the soil.

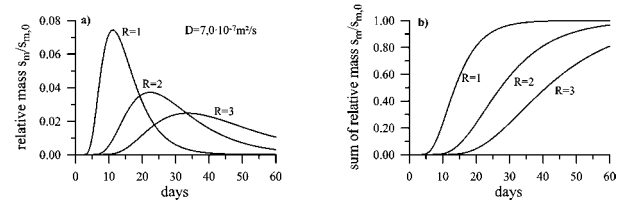


figure 7: influence of retardation/sorption on an impulse on top of a column

Internal reactions (decay and/or degradation) may be described as zero or first order process as shown in figure 8.

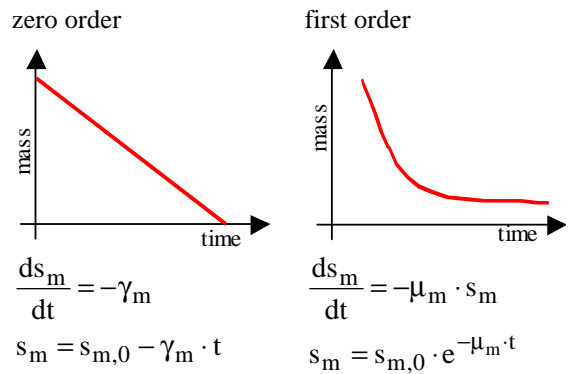


figure 8: order and description of degradation processes

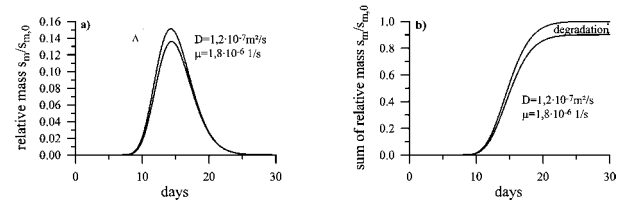


Figure 9: influence of degradation on breakthrough curves

BOUNDARY CONDITIONS AND PARAMETERS

Flow Model

The column has a height of 3.80 m, which corresponds to the groundwater table taken from Figure 2. The groundwater is the lower boundary condition, it is a first kind boundary condition of eq. (1). The flux difference between precipitation and evapotranspiration is applied as second type boundary condition at the top of the column. This is actually a transient boundary condition as shown in Figure 10.

Using transient flow conditions results in a very large the computig time. Therefore it is a common simplification to assume steady-state flow conditions with a mean recharge rate. But a proof is needed, if there are no differences in the results.

The space discetization of the column was held constant with $dz=0.01$ m. Each of the soil layers needs to be de-

scribed in its hydraulics with 5 parameters. Their values were taken from the field soil description and available soil data bases, like UNSODA (Schaap et al. 1999). The chosen parameter values are listed in Table 1.

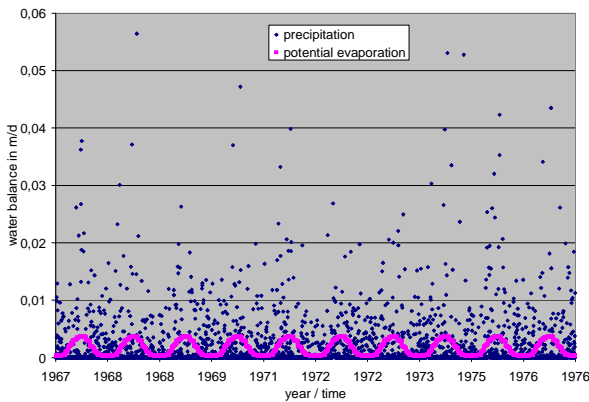


Figure 10: Precipitation and Potential Evaporation vs. Time

Table 1: Soil Hydraulic Parameters

parameter	symbol	dimen- sion	infilling	coarse middle sand	silty middle sand
porosity	ϕ		0.36	0.35	0.38
residual wa- ter conetent	$\theta_{w,r}$		0.09	0.07	0.1
scale factor	α	1/m	0.8	1.0	1.0
slope factor	n		2.0	2.0	2.0
hydraulic conductivity	k_f	m/s	$1 \cdot 10^{-4}$	$1 \cdot 10^{-3}$	$5 \cdot 10^{-4}$
bulk density	ρ	kg/m ³	1.700	1.700	1.700
dispersivity	δ	m	0.5·GWFA		

legend: GWFA – groundwater level below surface

Transport Model

The source chromate concentration at the top of column was chosen to 30 mg/l, starting from $t=0$ to $t=20$ a. The remaining parameter is the distribution coefficient to describe the sorption and retardation of chromate in the unsaturated zone. More than 42 drillings were done at the site. From these 42 drilling more than 100 samples were taken and analyzed for their chromium and chromate content in the soil and in the leachate. So it should not be a problem to establish a relation between the chromate content in the soil and in the liquid. But there is still a lack of methods and understanding. Right now it is known, that the measured chromate content in the liquid is not to compare with an actual leachate concentration in the field scale. So we had to do, what we always do in such cases, we searched in the literature for similar cases and found some hints for chromate retardation coefficients. From there we calculated the distribution coefficients using eq. (5) to $K_D=1,3 \cdot 10^{-3} \text{ m}^3/\text{kg}$, $R \approx 6$.

SCENARIOS

The defined cases distinguish between simplification of basic equations and parameter models and sensitivity calculations for parameter values.

Case 1 is the basic case. It is defined as a transient simulation of water flow and solute transport in the unsaturated zone for our contaminated site.

Commonly used simplifications of equation (1) are

case 2: the neglectation of storage terms, which results in steady-state conditions with a mean groundwater recharge rate as given flux instead of a transient flux

case 3: gravity driven flow processes, this case is actually not physically based and will not be regarded any further

A further commonly used simplification of the model of the subsurface is

case 4: a homogeneous unsaturated zone

The cases for sensitivity analysis are defined as

case 5: variation of the leachate rate (=groundwater recharge rate) in the range $v_N=178 \text{ mm/a} \pm 20\%$

case 6: variation of the saturated hydraulic conductivity in the range $5 \cdot 10^{-4} \leq 1 \cdot 10^{-3} \leq 5 \cdot 10^{-3} \text{ m/s}$

case 7: variation of the scale factor α from eq. (2) in the range $0.5 \leq 1.0 \leq 2.0 \text{ 1/m}$

case 8: variation of the slope factor n from eq. (2) in the range $1.5 \leq 2.0 \leq 3.0$

case 9: variation of the residual water content θ_r from eq. (2) and (3) in the range $0 \leq 0.07 \leq 0.1$

case 10: variation of the porosity ϕ from eq. (2), (3) and (5) in the range 0.35 ± 0.05

case 11: variation of the sorption coefficient K_D from eq. (4) and (5) in the range $5 \cdot 10^{-4} \leq 1 \cdot 10^{-3} \leq 5 \cdot 10^{-3} \text{ m}^3/\text{kg}$

case 12: variation of the source concentration c_0 in the range $25 \leq 30 \leq 50 \text{ mg/l}$

case 13: variation of the dispersivity δ from eq. (4) in the range $0.5 \leq 1.0 \leq 2.0 \text{ m}$

The case 14 “variation of degradation rate μ_n from eq. (4)” could not be analyzed, because chromium/chromate is not degradable.

Please note there are no cases defined to investigate simplifications of the convection-dispersion-equation (2). There must not be any simplification, because all of incorporated processes must be taken into account to get an appropriate concentration forecast.

Case 2 is the most commonly used simplification for leachate forecasts. The results of all other cases will be compared with the results of case 2.

The flow problem is solved if the recharge rate at the top of column is given (=case 2). Therefore one may not expect, that the results of cases 6-10 will differ significantly to the result of case 2. The mean recharge rate is given with $0.178 \text{ m/a} = 5.6 \cdot 10^{-9} \text{ m/s}$. This value is as the functions in Figure 11 show much more smaller than the

saturated and also the unsaturated hydraulic conductivity of used materials. The water content of these materials is always greater than the residual water content, therefore the given recharge rate can be flow through the unsaturated zone without any resistance. Please note, that we have much more higher recharge rates under transient conditions. They may be greater than the saturated hydraulic conductivity. In this cases runoff occurs at the surface, the soil is saturated and not able to receive more water. The storage capacity (represented with the parameters ϕ , $\theta_{w,r}$, α and n , cases 7 - 10), is neglected anyway. But there might be a small influence of the parameters α and n because of the incorporation of the water content in eq. (4). This may influence the migration velocity too. This statement also meets the parameters ϕ , $\theta_{w,r}$, which have an influence to eq. (2) via the calculation of the water content from eq. (1b).

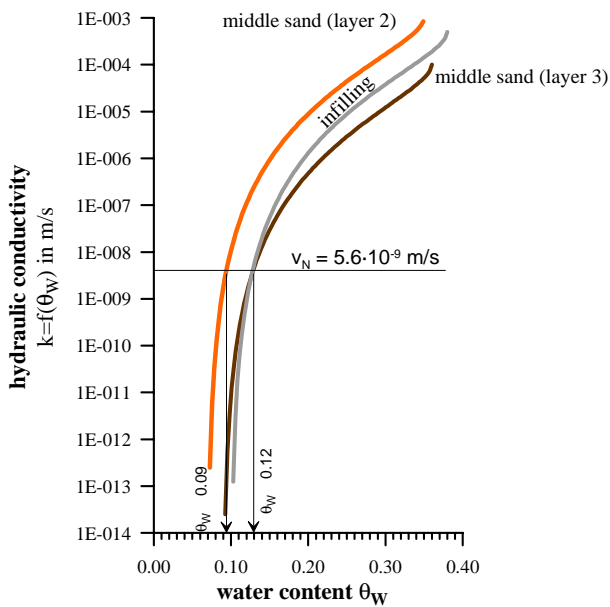


Figure 11: hydraulic conductivity function of used materials

RESULTS

The computational results of the basic case 1 are shown in Figure 12. The highest chromate concentration in the solute will be about 25 mg/l at $t=24$ a. This results meets the observations, which were done in the 90-ies. The concentration descends after the peak went through, because the source was removed in the beginning of the 90-ies. Within the regarded 100 years about 110 g/m² chromate will reach the groundwater.

The highest yield occurs after 22 years with 105 g/a. This amount is caused by a high but shortterm flux rate. The results for all other cases are listed in Table 2. The columns contain

1. the highest chromate-concentration c_{max} ,
2. the time of its occurrence,
3. the amount of highest yield Y_{max} ,

4. the time of its occurrence and
5. the total chromate mass within 100a, reaching the groundwater per m².

The comparisn of results from case 1 to case 2, shows that there is no need for transient flow conditions, the calculated concentration, yield, mass and times of occurences are always close together or identical.

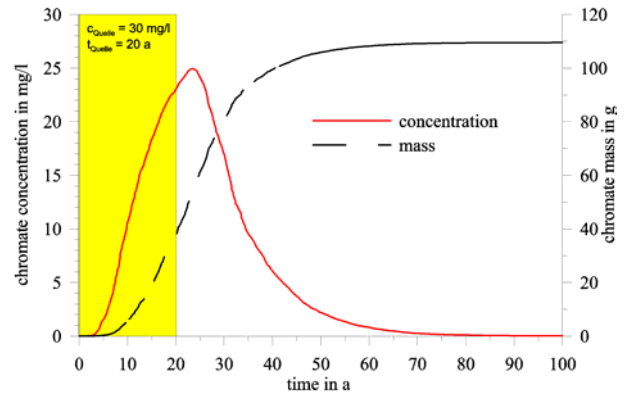


Figure 12: calculated chromate concentration and sum of chromate mass vs. at the bottom of the column

Table 2: Calculated Results

case	concentration		yield		sum of mass
	c_{max}	year	Y_{max}	year	m
	mg/l	a	mg/a	a	g
1	24.9	24	105000	22	110
2	24.5	24	4242	24	105
3	1.5	100	269	100	7
4a	24.5	24	4238	24	105
4b	24.6	24	4263	24	105
4c	24.5	24	4235	24	105
5a	26.4	23	5481	23	125
5b	22.1	25	3053	25	85
6a	24.7	24	4263	24	105
6b	24.7	24	4263	24	105
7a	25.0	24	4302	24	105
7b	24.4	24	4225	24	105
8a	24.9	24	4291	24	105
8b	24.5	24	4238	24	105
9a	24.6	24	4253	24	105
9b	24.8	24	4288	24	105
10a	24.5	24	4235	24	105
10b	24.8	24	4291	24	105
11a	17.0	30	2935	30	> 105
11b	28.8	21	4982	21	105
12a	32.9	24	5684	24	140
12b	16.4	24	2842	24	70
13a	26.5	22	4581	22	105
13b	24.7	27	4262	27	105

The case 3 is as mentioned above an exception. It is not acceptatable to reduced the flow conditions to a gravity

driven flow by a given first flux boundary condition at the bottom.

The cases 4a, b and c are defined by a homogeneous soil column. The results show, that there is also no significant difference to the results of case 2. The soil hydraulic parameters k_f (case 6), the van-Genuchten-Parameters α , n (case 7, 8), the porosity ϕ and residual water content $\theta_{w,r}$ (case 9, 10) also do not have too much influence on the results. Significant differences are calculated with slight changes in the mean groundwater recharge rate and all transport parameters.

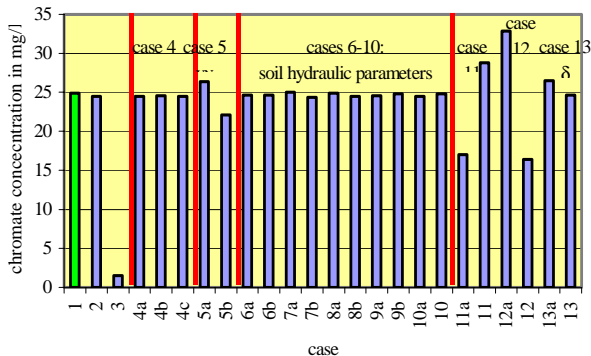


Figure 13: calculated concentrations at the bottom of the column

CONCLUSIONS

The results of the scenario and sensitivity analysis showed the thesis, that

- ✓ it is acceptable to assume steady state flux conditions over a long term period instead of using a transient precipitation boundary condition
- ✓ the soil hydraulic parameters do not influence the calculated concentration at the bottom of a column, if their order of magnitude was quite real estimated

During parameter identification the

- ✓ groundwater recharge rate
- ✓ source concentration and
- ✓ distribution coefficient

must be determined as accurately as possible.

But these statements are only valid, if the hazard is not degradable. Further investigations will be done on organic contaminations like a fuel depot. First calculations have shown, that the calculated concentration is highly related to the given transient flux conditions due to the degradation. A systematization scheme must be developed.

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ACKNOWLEDGEMENTS

This research work was granted by the German Department of Education and Science (BMBF-Bundesministerium für Bildung und Forschung) contract # 02WP 0192, 0242, 0502 and 0503.



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