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Simple models for reactive transport of pollutants and main constituents during artificial recharge and bank filtration

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ABSTRACT: As an alternative to reactive transport codes which require a high skill and tedious data input, 2 simple models are presented for use in artificial recharge and bank filtration. INFOMI is a finite element 1D-model using 'mixing cells in series'. It incorporates: a variable input signal; volatilization and breakdown in the infiltration basin; filtration of pollutants attached to suspended particles; and advection, dispersion, sorption and breakdown in the saturated zone. EASY-LEACHER is a 2D spread-sheet model, based on: the mass balance approach; travel times derived from a separate hydrological model; and empirical rules on reaction sequence and kinetics. The model simulates: the displacement of native groundwater; the leaching of exchangeable cations, calcite, organic matter and iron sulphides; the breakthrough of reactive solutes; and sorption and breakdown of micropollutants. The behaviour of 4 radionuclides and trihalomethanes upon artificial recharge is predicted using INFOMI. Quality changes of injected surface water when recollected by a distant well, are calculated by EASY-LEACHER.

1 INTRODUCTION

Modelling the water quality changes of surface water during detention in spreading basins and/or during aquifer passage can contribute in various ways to the design, optimization and monitoring of systems with artificial recharge (AR) or bank infiltration (BI). Important questions to be solved are: (a) which system is to be preferred from a chemical point of view (BI or AR using either basins or deep wells)?; (b) which is the minimum detention time required for removal of specific pollutants?; (c) which aquifer is best suited to eliminate for instance nitrate, nickel, atrazin and trihalomethanes?; (d) which parameters can be used to screen the analytical program?; and (e) on which time scale is oxygen in the influent reaching the recovery well and then triggers the clogging process?

The current generation of complex reactive transport models like PHREEQC (for an application in MIKE-SHE see Brun et al. 1998) and the future generation which will be integrated with geographical information systems (Griffioen et al. 1998), are in a way handicapped. They require a very detailed data entry, long computation times (or powerful computers) and an extremely high skill of the performer. This provoked the development of 2 simple reactive transport models at Kiwa, INFOMI 3.1 (Dijkhuis & Stuyfzand 1996) and EASY-LEACHER (Stuyfzand in prep).

2 INFOMI

INFOMI is the acronym for 'INFiltration Of MIcropollutants'. It is a finite element 1D-model using the 'mixing cells in series' concept, incorporating (Fig.1): (a) a highly variable input signal for the pollutants in surface water; (b) in the infiltration basin or in a specific river segment: volatilization, photochemical and microbiological first order breakdown; (c) at the water/sediment interface: filtration of pollutants attached to suspended particles; and (d) in the saturated zone: advection, dispersion (plus diffusion), linear sorption (including DOC as a carrier), and first order breakdown (organics and radionuclides).

Some general specifications are given in Table 1, and the most important transport equations are collected in Table 2. Advection and dispersion (+diffusion) in the aquifer system are modelled using algorithms of Appelo & Postma (1993). A flow path is essentially subdivided into at least 3 parts (Fig.1): (1) the infiltrating water course, (2) the water/sediment interface, and (3) the aquifer system, which may be further subdivided, for instance into bottom sludge or an upper aquiclude and the aquifer. The concentration which is calculated for the exit of each compartment, forms the input for the next compartment.

Standard the model generates the concentration in the aquifer along the flow path (distance travelled), and the concentration with time (the breakthrough curve) on each desired point along the flow path within the aquifer. Variables which need to be known, are specified in Table 2. The most important assumptions or conditions of the model are: (1) suspended solids are filtrated at the water/sediment interface and do not play a further role, because of inert behaviour or removal by either erosion or sludge scraping; (2) steady hydrology (travel times, water depth in ponds, flow path, etc.); (3) there is no unsaturated zone; (4) each soil compartment is homogeneous and geochemically in steady state (no changes in redox environment and in leaching or accumulation of reacting components); (5) no DOC-accelerated transport of organic pollutants (see also 8); (6) trace metals are only influenced by sorption (no precipitation/dissolution); (7) each decay process is first-order (one T½); (8) the flow velocity and longitudinal dispersivity (α_L) are constant within each soil compartment; (9) linear, reversible sorption without competition; and (10) there is no temperature dependency, except for volatilization.

Table 1. Comparison of characteristics and performance of two simple models dveloped at Kiwa.

item	INFOMI 3.1	EASY-LEACHER
water quality[1]	OMPs, TMs	MCs, OMPs
dimension	1-D (2-D)	2-D (3-D)
input signal	all	step[@]
processes considered:		
•in water course[2]	vol, phot, bio	-
•at water/sed. interface	filtration	filtration
•within aquifer system[3]	advect., disp, sorp., decay	as INFOMI 3.1 + leaching[4]
hardware	PC, ≥486	PC, ≥486
software	Turbo-Pascal	spread-sheet QPRO

1: OMPs = Organic MicroPollutants; TMs = Trace Metals; MCs = Main Constituents

2: vol = volatilization; phot = photolysis; bio = biodegradation

3: advect = advection; disp = dispersion (incl. diffusion); sorp = sorption

4: including: cation exchange, oxidation of pyrite and organic matter, and calcite and MnO_2 dissolution.

@: stepwise change from native situation to artificial recharge or bank filtration (with mean recharge composition).

3 EASY-LEACHER

EASY-LEACHER is an analytical 2D-spread sheet model (Fig.2). It is based on: (a) the mass balance approach, for both reactive solutes in the water recharged and solid reactive phases in the aquifer system; (b) the cumulative frequency curve of detention times for a well or well field as derived from a separately run hydrological model; and (c) some empirical rules regarding the sequence of reactions and reaction kinetics. The model simulates for as many strata as desired: (a) displacement of the native groundwater by the water recharged; (b) the leaching of reactive soil constituents: exchangeable cations, calcite, organic matter and iron sulphides; (c) the breakthrough of reactive solutes; and (d) sorption and breakdown of organic micropollutants.

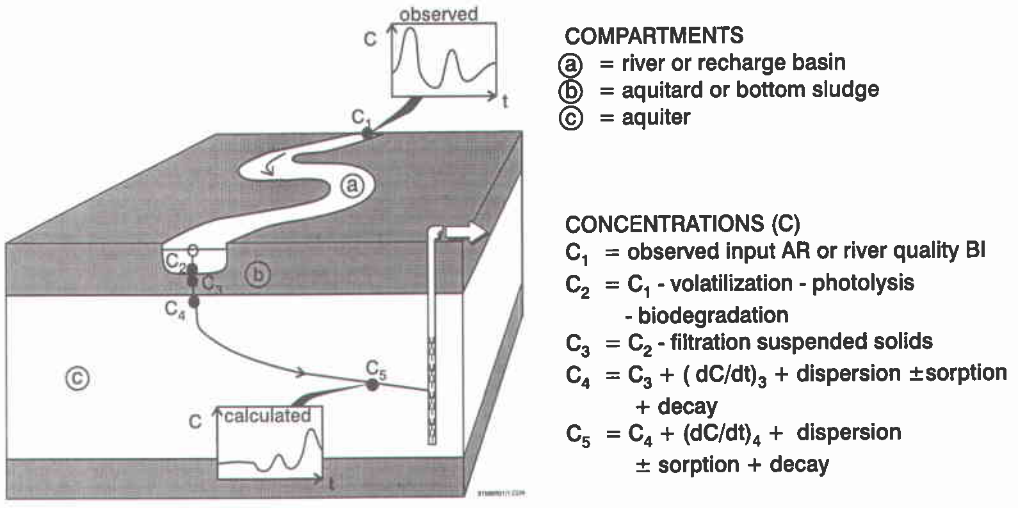


Figure 1. Essential features of INFOMI 3.1.

Table 2. The most important transport equations (hydraulics excluded) used in INFOMI 3.1

Volatilization, photolysis and biodegradation in a recharge basin or river segment
Assuming simultaneous decay and first order decay rates for all 3 processes, we obtain:

$$C_{t_i} = C_o e^{-(\lambda_v + \lambda_p + \lambda_b)t_i} \tag{1}$$

with:
λ_v, λ_p, λ_b = ln(2)/T½ = decay constant of OMP during resp. volatilization, photolysis and biodegradation [1/d]; (T½) = half life during resp. volatilization, photolysis and biodegradation [d]; t_i = travel time in infiltrating water course [d]; C_0 = initial concentration [mol/L]; C_{ti} = concentration after t_i days [mol/L].
Volatilization is calculated using the approach of Southworth (1979) with estimation of transport coefficients according to McKay & Shiu (1981), and with correction for TOC-binding. Combination yields:

$$\lambda_v = \frac{8.995\,10^{-3} K_H}{(1.68\,10^{-3} K_H + 6.18\,10^{-5} T)(1 + K_{oc} TOC\,10^{-6}) D_{sw} \sqrt{M}} \tag{2}$$

with:
K_H = constant of Henry [Pa.m^3/mol]; T = absolute temperature [K]; D_{sw} = mean water depth of infiltrating water course [m]; M = Molecular weight of organic micropollutant [g/mol]; TOC = Total Organic Carbon in surface water [mg C/L]; K_{oc} = distribution coefficient between organic carbon and water [L/kg C].
If K_{oc} is unknown, calculate by:
$K_{oc} = 10^b K^a_{ow}$, with K_{ow} = octanol water distribution coefficient, a and b = regression parameters (see Appelo & Postma 1993); or $K_{oc} = 10^{3.64}\ S^{-0.55}$ with S = solubility OMP in water [mg/L].

Filtration at the water/sediment interface
Analytical results of OMPs in surface water generally refer to total concentrations. Assuming that all sorption to suspended particles occurs to particulate organic carbon (POC = TOC - DOC), and that POC-binding forces equal TOC-binding forces, yields (Stuyfzand & Lüers 1996):

$$OMP_{diss} = OMP_{tot}\left(\frac{DOC}{TOC} + \frac{1 - (DOC/TOC)}{1 + K_{OC} TOC\,10^{-6}}\right) \tag{3}$$

with:
DOC = Dissolved Organic Carbon in surface water [mg/L]; OMP_{tot} = total concentration of Organic Micro-Pollutant [µg/L]; OMP_{diss} = concentration of dissolved OMP = free + DOC-bound [µg/L].
The fraction removed by filtration then equals:
$(OMP_{tot} - OMP_{diss})/OMP_{tot}$

Sorption of organic micropollutants within the aquifer system
Retardation due to sorption is calculated using the classical approach (see Appelo & Postma 1993) with addition of the effects of DOC-binding according to Kan & Tomson (1990) and of dissociation according to Schellenberg (1984):

$$R = \left(1 + \frac{\rho_b f_{oc} f_{nd} K_{oc}}{n(1 + f_{nd} TOC\,10^{-6} K_{oc})}\right) \tag{4}$$

with:
ρ_b = bulk density of aquifer matrix [kg/L] = (1-n)ρ_s with ρ_s = density of solids in aquifer matrix = 2.65 kg/L; n = porosity [L/L]; f_{oc} = fraction organic carbon in aquifer matrix [-]; $f_{nd} = 1/(1 + 10^{pH-pKa})$ = correction for dissociation, which is important only if K_{oc} or K_{ow} were measured at pH_{exp} < pKa and pH (= pH_{sample}) > pH_{exp}; $pK_a = -\log K_a$, with K_a = first dissociation constant of H-OMP.

Sorption of trace metals within the aquifer system
If calcium is the main cation sorbed to the aquifer matrix, then the retardation of trace metal M can be calculated as follows:

$$R = 1 + \frac{\rho_b CEC}{nm}\left(K_{M\backslash Ca}\frac{\beta_{Ca}^{0.5}}{[Ca^{2+}]^{0.5}}\right)^m \tag{5}$$

with:
CEC = actual Cation Exchange Capacity = Na_{EXCH} + K_{EXCH} + Ca_{EXCH} + Mg_{EXCH} + NH_{4EXCH} + ... [meq/kg dry weight]; $K_{M\backslash Ca}$ = exchange constant (using the Gaines-Thomas convention) for metal M^{m+} in equilibrium with Ca^{2+} [-], according to the reaction: 1/m M^{m+} + ½Ca-$EXCH_2$ ↔ 1/m M-$EXCH_m$ + ½Ca^{2+} . This constant is calculated from $K_{Na/M}$-values listed in Appelo & Postma (1993), by taking: $K_{M\backslash Ca} = (K_{Na/Ca} / K_{Na/M})$; β_{Ca} = fraction of calcium in CEC of aquifer matrix = Ca_{EXCH}/CEC [-]; m = charge of metal M; [Ca^{2+}] = total calcium concentration infiltration water [mmol/L].

Degradation or radio-active decay is calculated using:

$$C_t = C_0 e^{-(\lambda_b t R)} = C_0 / 2^{\frac{tR}{(T_{1/2})_b}} \tag{6}$$

with:
t = travel time of water in aquifer system [d]; T½ = half life due to biodegradation (depends on redox etc.) or radio-active decay [d]; R = retardation factor, Eq.4 for OMPs and Eq.5 for trace metals.

Contrary to most transport codes, the situation after each time step is directly calculated with analytical formulae, without iterations, finite elements and equilibrium calculations (calcite excluded).

In contrast to INFOMI 3.1. the composition of the recharge water is assumed constant, and the leaching of reactive solid phases is accounted for. The latter is essential for both the major constituents and organic pollutants (where the advance of redox zones determines the overall breakdown).

Some general specifications are given in Table 1, and some of the most important transport equations regarding inorganics are collected in Table 3. The equations regarding organic micropollutants are equal to those listed in Table 2. The transport equations involving calcite dissolution and the oxidation of organic matter strongly depend on the leaching sequence.

As shown in Fig.2 there are essentially 2 options for running EASY-LEACHER. When flow parallels the discerned aquifer layers, as in case of deep well injection, the model is built up by the individual layers. If flow crosses the discerned aquifer layers, as in case of basin recharge, the model is built up by selected flow paths. In the latter case some problems may arise and information on the exact position of leaching fronts is lost, due to the necessity to average the geochemistry along each flow path (excluding sludge at the bottom of recharge basins, which is treated separately).

The assumptions or conditions of the model are the same as those mentioned for INFOMI 3.1, excluding number 4 (each soil compartment can be leached here). Additional assumptions are: (a) bottom sludge in a recharge basin remains in steady state leading to constant O_2 and NO_3^- losses by oxidizing organic material; (b) DOC and NH_4^+ in the water recharged are first partly oxidized, the remaining O_2 and NO_3^- can oxidize aquifer materials; (c) exchange reactions and the dissolution of inorganic aquifer phases are without kinetic hinderance (sharp fronts); (d) the leachable phases are all homogeneously distributed within each layer or along each flow path; (e) organic material in the aquifer matrix is composed of a labile (highly reactive), tough (little reactive) and inert fraction, with the tough fraction being oxidized only after total consumption of the labile fraction; (f) the oxidation rate of organic material depends on the presence of O_2 and NO_3^-, and the original amount of the labile c.q. tough fraction; and

(g) the leaching sequence is such that when pyrite is completely leached, tough organic material is still present.

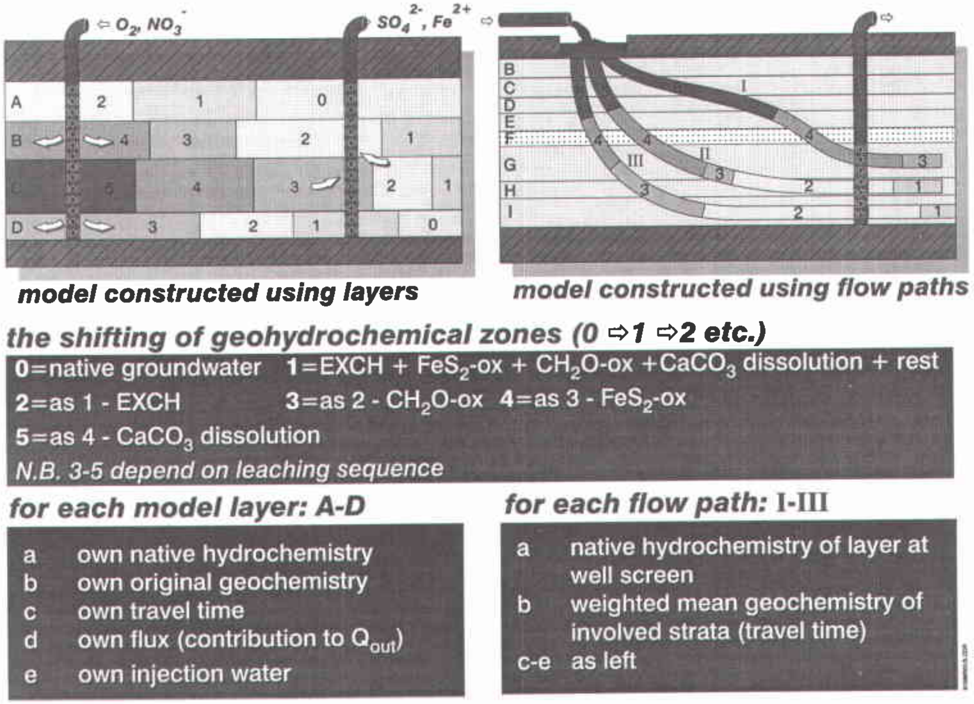


Figure 2. Essential features of EASY-LEACHER in case flow parallels the stratified medium (left) or crosses it (right).

Table 3. Some of the most important transport equations used in EASY-LEACHER.

The retardation and leach factor in general
Sorbing and oxidizing solutes are retarded during aquifer passage, and similarly desorbing and dissolving compounds are delayed by leaching. In the latter case raised concentrations drop to the influent level long after passage of the chloride - front. These delays are quantified by respectively the retardation factor R_i and leach factor L_i:

$$R_i = \frac{t_i}{t_{H2O}} \qquad (7.1) \qquad\qquad L_i = \frac{t_L}{t_{H2O}} \qquad (7.2)$$

with: t_i = time for 90% breakthrough of solute "i" [days]; t_L = time required for 90% leaching or till equilibrium is attained with the injection water [days]; t_{H2O} = mean travel time for water or a conservative tracer like chloride [days].
For practical reasons 90 in stead of 100% breakthrough or leaching has been chosen.
The general formula for a stationary and fast leaching of a homogeneously distributed reactive phase in the aquifer, is:

$$L = 1 + \frac{\rho_b(solid)}{n(reac)r_r} \qquad (8)$$

with: (solid) = content of reactive phase in aquifer [mmol/kg dry weight]; (reac) = concentration of reactant in flushing fluid [mmol/L]; r_r = reaction coefficient, i.e. number of mmoles of solid phase leached by 1 mmol of reactant [-].
In stead of the concentration of the reactant (reac) and its reaction coefficient r_r, also the concentration of a reaction product (prod) and its reaction coefficient r_p can be taken, so that Eq.8 becomes:

$$L = 1 + \frac{\rho_b(solid)}{n(prod)r_p} \qquad (9)$$

Of course, (reac) or (prod) should have no other sinks or sources, unless these can be properly accounted for.

Cation exchange
The period of cation exchange reactions (here Base EXchange) can be estimated by:

$$R_{BEX} = L_{BEX} = 1 + \frac{\rho_b CEC}{n\Sigma c} \qquad (10)$$

with: CEC = cation exchange capacity [meq/kg d.w.]; Σc = sum of cations in flushing liquid, the influent [meq/L].
For the individual, adsorbed cations like Fe^{2+}, Mn^{2+} and NH_4^+ the following approximation holds:

$$L_{X\text{-}EXCH} = 1 + \frac{\rho_b X_{EXCH}}{0.75 n X_O} \qquad (11)$$

with: X_{EXCH} = content of X in cation exchange complex [meq/kg d.w.]; X_O = concentration of X in native groundwater prior to displacement [meq/L]. The factor 0.75 is empirical and assumes the water recharged to be without X.

Pyrite oxidation
The leach factor for pyrite (FeS_2) is the result of oxidation by O_2 and/or NO_3^-:

$$L_{FeS2} = 1 + \frac{\rho_b(FeS_2)}{0.5n(\Delta SO_4)} \qquad (12)$$

with: (FeS_2) = pyrite content [mmol/kg d.s.]; ΔSO_4 = sulphate-increase due to pyrite oxidation [mmol/L].

4 INFOMI APPLIED TO RADIONUCLIDES

4.1 *Definition of the problem*

The behaviour of ^{90}Sr, ^{60}Co, ^{106}Ru and ^{137}Cs during dune sand passage was modelled after basin recharge without interfering sludge layer. Hypothetical, relatively short pulses (of 1-28 days) with 100% activity were chosen as input signal, in order to simulate a calamity at the recharge facility of The Hague (using spreading basins).
System parameters for the aquifer were:
$n = 0.38$, $\rho_s = 2.65$ [kg/L], $\alpha_L = 1$ m; $D = 4\ 10^{-5}$ m^2/d; CEC = 20 meq/kg; $Ca_{EXCH} = 17$ meq/kg ($\beta_{Ca} = 0.85$); length of flow path = 70 m; cell size = 1 m; $v_{H2O} = 1$ m/d; Ca-infiltrate = 2 mmol/L.
Characteristics of the radionuclides are (partly after Haberer 1989): $K_{Co/Ca} = 0.67$; $K_{Sr/Ca} = 1.14$; $K_{Ru/Ca} = 1.14$; $K_{Cs/Ca} = 3.43$;
$(T½)_{Co} = 1925$ d; $(T½)_{Sr} = 10483$ d; $(T½)_{Ru} = 368$ d; $(T½)_{Cs} = 10958$ d.

4.2 *Strontium-90*

The propagation of the ^{90}Sr-pulses along a representative 70 m long flow path in dune sand is shown in Fig.3. The duration of the calamity has a strong impact on the final radio-activity along the flow path. Due to a relatively slow radio-active decay and little retardation, strontium activities remain significant in the recovery well. Radiostrontium breaks through there after about 2 years and it takes 2-2.5 years to flush it from the aquifer. A maximum activity of 0.5% is calculated for a pulse of ½ week and of 6% for a pulse of 4 weeks. Mixing in the recovery well is expected to reduce the activities by about 50%.
As radiostrontium is hardly removed by post-treatment, radiostrontium poses a health hazard which requires a save fluvial alarm system and cautious selective intake system.

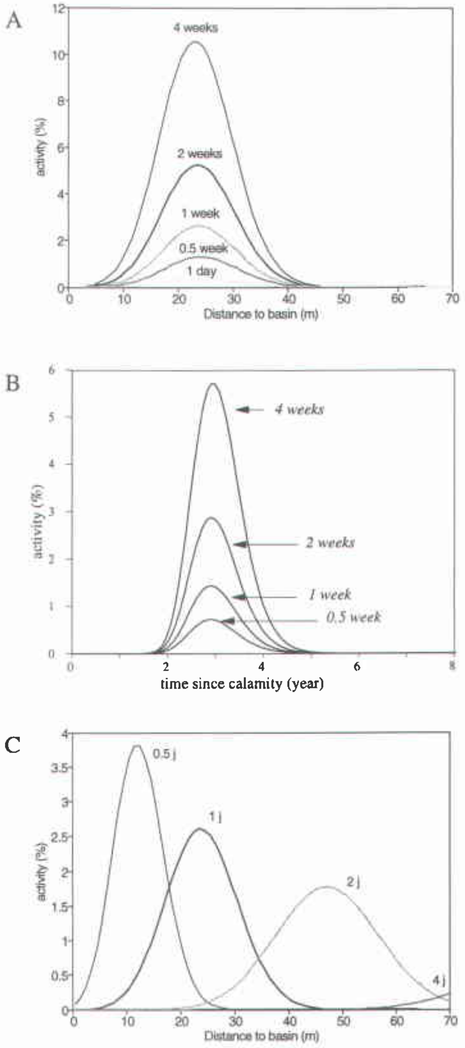


Figure 3. Simulated behaviour of radioactive strontium-90 during passage of dune sand in a basin recharge system, in case of a calamity (pulse) of resp. 1 day, ½, 1, 2 and 4 weeks. A: concentration along a flow path 1 year after the start of the calamiy. B: concentration at the end of the flow path (70 m) in the recovery well (breakthrough curve). C: propagation of a 4-weeks pulse along the flow path. v_{H2O} = 1 m/d; α_L = 1 m. R_{Sr} = 15.7; $(T½)_{Sr}$ = 28.7 year.

4.3 ^{60}*Co*, ^{90}*Sr*, ^{106}*Ru and* ^{137}*Cs*

The breakthrough of a combined ^{60}Co-, ^{90}Sr-, ^{106}Ru- and ^{137}Cs-puls of 1 week at the end of a 70 m long flow path in dune sand is shown in Fig.4. Differences in retardation clearly lead to peak separation: ^{60}Co (R = 6.1) arrives first after 0.5 year, after about 2 years ^{90}Sr and ^{106}Ru (R = 15.7) follow, and ultimately after 10 years ^{137}Cs (R = 133.8) appears. Again, 100% was the starting activity for each radionuclide upon infiltration. Filtration and precipitation were not considered, which makes the approach for cobalt, ruthenium and especially cesium a true worst-case scenario. Strontium, however, is hardly subject to these processes so that its results may approach reality.

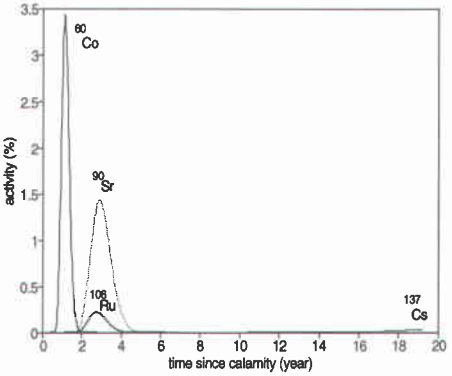


Figure 4. Breakthrough curves for radio-active cobalt-60, strontium-90, ruthenium-106 and cesium-137 after 70 m passage of dune sand in a basin recharge facility, in case of a calamity (pulse) of 1 week. v_{H2O} = 1 m/d; α_L = 1 m. R_{Co} = 6.1; $R_{Sr} = R_{Ru}$ = 15.7; R_{Cs} = 133.8; $(T½)_{Co}$ = 1925 d; $(T½)_{Sr}$ = 10483 d; $(T½)_{Ru}$ = 368 d; $(T½)_{Cs}$ = 10958 d.

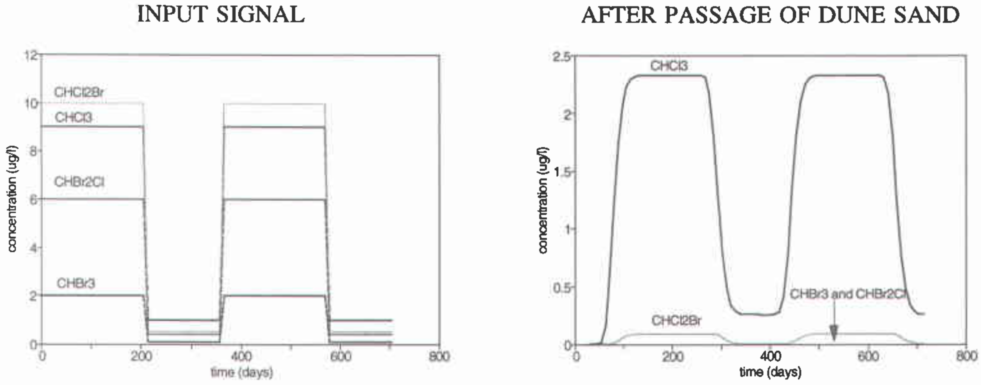
5 INFOMI APPLIED TO TRIHALOMETHANES

5.1 *Definition of the problem*

The behaviour of chloroform ($CHCl_3$), bromodichloromethane ($CHCl_2Br$), dibromochloromethane ($CHBr_2Cl$) and bromoform ($CHBr_3$) was simulated for a basin recharge system. The system implies subsequently: (a) 2 days detention in a recharge basin (volatilization and biodegradation in oxic environment); and (b) 70 m transport in dune sand (convective transport, dispersion, sorption and degradation in (sub)oxic environment).

The 2 years input signal is composed of a pulse during the period April - October (214 days), when chlorination for transport occurred. Peak and background levels were resp. 9 and 1 µg/l for chloroform, 10 and 0.5 µg/l for $CHCl_2Br$, 6 and 0.4 µg/l for $CHBr_2Cl$ and 2 and 0.1 µg/l for bromoform.

System parameters for the recharge basin are: residence time = 2 d; water temperature = 17°C; water depth = 1.5 m. System parameters for the sand aquifer are: n = 0.38, ρ_s = 2.65 [kg/L], α_L = 1 m; D = $4 \cdot 10^{-5}$ m^2/d; f_{OC} = 0.001; TOC-infiltration water = 4.2 mg/l; (DOC/TOC)-infiltration water = 0.85; DOC-infiltrate = 2.8 mg/l; length of flow path = 70 m; cell size = 1 m; v_{H2O} = 1 m/d.


INPUT SIGNAL

AFTER PASSAGE OF DUNE SAND

Figure 5. Input signal for trihalomethanes in pretreated water, and the calculated concentrations after a 2 days detention in the recharge basin and after passage of 70 m of dune sand. The input signal contains recurring pulses of 7 months due to transport chlorination in the period April - October. v_{H2O} = 1 m/d; α_L = 1 m. Concentration in the basin is lowered by about 50% for each THM. In dune sand: $R_{CHCl3} = 1.17$; $R_{CHCl2Br} = 1.5$; $R_{CHBr2Cl} = 1.77$; $R_{CHBr3} = 2.19$.

Characteristics of the OMPs are:
for chloroform: K_H = 304 Pa m^3/mol; $(T½)_b$ = 80 d; log K_{OC} = 1.6; M = 119.4 g/mol.
for $CHCl_2Br$: K_H = 162 Pa m^3/mol; $(T½)_b$ = 17 d; log K_{OC} = 2.07; M = 163.8 g/mol.
for $CHBr_2Cl$: K_H = 88 Pa m^3/mol; $(T½)_b$ = 4.5 d; log K_{OC} = 2.26; M = 208.3 g/mol.
for bromoform: K_H = 44 Pa m^3/mol; $(T½)_b$ = 3 d; log K_{OC} = 2.44; M = 252.7 g/mol.

5.2 *Results*

A 2 days detention in a recharge basin leads to a reduction of each THM by about 50%, mainly due to volatilization and little by biodegradation. The passage of 70 m of dune sand in (sub)oxic environment raises the retardation and degradation in the following order: chloroform < dichlorobromomethane < dibromochloromethane < bromoform. Only chloroform and some dichlorobromomethane 'survive' the aquifer passage (Fig.5). These calculations correspond well with observations (Stuyfzand 1989).

6 EASY-LEACHER APPLIED TO DEEP WELL INJECTION

6.1 *Definition of the problem*

The water quality evolution in the recovery well of deep well injection experiment number 11 (Stuyfzand 1998) was simulated using EASY-LEACHER. Pretreated oxic water from the Zuid-Willemsvaart (a canal containing mainly river Meuse water) is injected into an anoxic Miocene sandy aquifer. Mean characteristics of the experiment are listed in Tables 1-2 of Stuyfzand (1998). The aquifer is schematized by 5 different horizontal strata (A-E), each with a different travel time, flux (contribution to the recovery well) and geochemistry (Table 4), and minor differences in native hydrochemistry (not shown). During the first year of the experiment the injection water reached the recovery well (at 98 m) in layers D and E only.

The most important reactions of the injected water with the aquifer matrix were, in decreasing order (Stuyfzand 1997): (a) pyrite oxidation in layers A-C exclusively by O_2, and in layers D-E by both O_2 and NO_3^-; (b) acid buffering by the injected HCO_3^- (converting to CO_2); (c) oxidation of labile organic material by nitrate (more in A-C than in D-E); (d) cation exchange, with especially Ca^{2+} and Na^+ expelling adsorbed Fe^{2+}, Mn^{2+} and NH_4+; (e) desorption of SiO_2; and (f) adsorption of F^-. These reactions were included in EASY-LEACHER.

6.2 *Results*

Some results of modelling the recharge experiment for 100 years are shown in Fig.6. Although the experiment had been running for only 1 year during our evaluation, measurements and model predictions can be compared over a much longer 'apparent' period, because the amount of pore flushes (similar to bed volumes) in monitoring wells closer to the injection well approach the amount of pore flushes after 100 years for the recovery well. In fact, there was satisfactory agreement (Stuyfzand 1997).

From Fig.6 some conclusions of practical interest were drawn. First, oxygen and nitrate are not expected to reach the recovery well within resp. 100 and 20 years, which reduces the risk on clogging of the recovery well by $Fe(OH)_3$ and bacteria due to mixing of aerobic and anaerobic water in and around the well screen. Second, a future water softening in the pretreatment is not expected to be counteracted by dissolution of $CaCO_3$, but a significant lowering of HCO_3^- should be avoided because this would reduce the internal buffering of acid produced by pyrite oxidation (and then lead to the mobilization of metals).

Table 4. Geohydrological and geochemical stratification of the Miocene target aquifer of deep well experiment 11 near Someren, the Netherlands.

model layer	unit	A	B	C	D	E
GEOHYDROLOGY						
depth top	m-MSL	248	253	266	270	280
depth base	m-MSL	253	266	270	280	287
permeability	m/d	4	12.5	5	17	25
travel time	d	1250	500	1000	300	200
flux#	%	3.2	27	3.2	27.8	28.8
GEOCHEMISTRY						
Fe_{EXCH}	meq/kg	1.61	0.26	1.12	0.15	0.06
Mn_{EXCH}	meq/kg	0.10	0.02	0.06	0.01	0.005
$NH4_{EXCH}$	meq/kg	0.04	0.02	0.03	0.02	0.01
$CaCO_3$	mmol/kg	0	0	0	0	0
C-organic	mmol/kg	1075	458	1150	167	113
FeS_2	mmol/kg	55.2	10.2	25.5	12.6	8.6

= permanent admixing of authochtonous groundwater is 10%

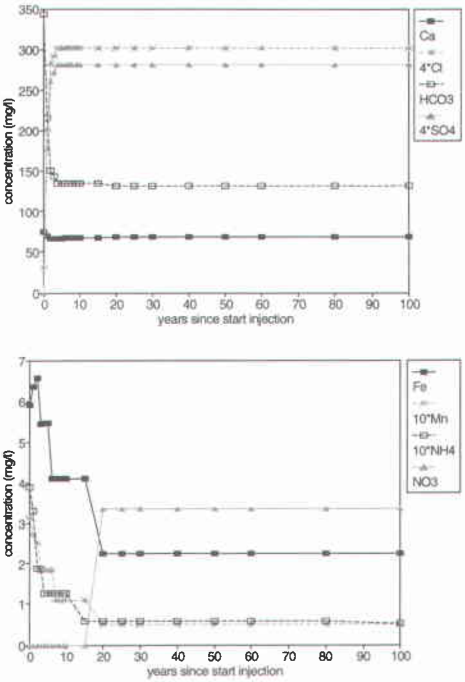


Figure 6. Quality development in the groundwater recovered at 98 m from the injection well of experiment 11, as predicted by EASY-LEACHER. Important input data for the model are listed in Table 4.

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