Hydrol. Earth Syst. Sci. Discuss., 8, C274–C285, 2011
www.hydrol-earth-syst-sci-discuss.net/8/C274/2011/

Hydrology and Earth System Sciences Discussions

Interactive comment on "Modeling subsurface transport in extensive glaciofluvial and littoral sediments to remediate a municipal drinking water aquifer" *by* M. Bergvall et al.

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Received and published: 4 March 2011

General Comments

The study describes field data and model simulation of the transport of the herbicide dichlobenil and its metabolite BAM (2,6-dichlorobenzoamide) through a 10-m deep vadose zone of a contaminated site and glaciofluvial esker aquifer in Northern Sweden. The vadose zone model HYDRUS-1D at point (i.e., soil profile) scale was coupled with the regional groundwater flow-transport model MODFLOW/MT3DMS. The vadose zone and aquifer was parameterized in the model using a combination of experimental or other independent information (soil profile data, geophysical data, pumping tests,

slug tests, stream bed leakage measurement, literature data, climate data, historical records) and model calibration. A sensitivity analysis was performed and revealed that the physical parameters infiltration rate and permeability of the aquifer were more sensitive than reactivity parameters related to sorption and degradation. The model simulation was used to suggest the optimal locations of two remediation wells, which were subsequently installed. The calibrated subsurface parameters permeability and specific yield could be validated using pumping tests at these remediation wells.

This is a case study on a simulation of pesticide transport through the vadose zone and sedimentary aquifer. For a pesticide modelling problem, the spatial and temporal scales are large (some 10 km2). The case study is part of a real groundwater remediation case. The approach was thoroughly conducted. The paper is well written and mostly well structured. Abstract and Introduction are very clear. For the other parts, some background information could be added (see below). The comparison between simulation and observed pumping test data and concentrations suggest a successful model application. However, after reading the paper I asked myself, what can we really learn from this study, for instance, about processes and their modelling at this scale? Partly this question may be caused by missing information. I will focus on the vadose zone modelling approach, since I found this less clear than the groundwater part:

(1) The vadose zone model was said to be assumed to represent the 'total open land area'. Figure 1 also gives the impression there was only one 1d-model for the entire domain. In reality there was pesticide input from the nursery and none from outside areas. If you apply a mixture (4% of 0.17 gm-2) for the total area instead of applying it only at the tree nursery area, this is a drastic deviation from the real situation! But looking at Fig. 6, simulated BAM does originate from the nursery. Please clarify in the text!

(2) Data of 5 measured soil profiles were mixed to give a representative soil profile. However, does that really represent average soil properties for the 'total land area' (see above)? How can this approach be justified? I think the calibration adjusted the

parameter of this profile, but this then will no longer represent any measured data, but an ‘effective profile’.

(3) The parameterization of the vadose zone: Was Ks measured? Indicate in Table 1 (e.g., using superscript symbols) which quantities were measured, which calibrated, and which represent literature estimates. Add dispersivities to Table 1.

(4) The role of the vadose zone modelling remains almost in the dark. The calibration gives some answers, but results for simulation and measurement should be shown also in terms of water contents and pesticide concentrations in the vadose zone.

(5) The beginning of the discussion of the results it is stated that a simpler approach leads to the same transit times for water and BAM. As it is now, the discussion is of limited value since the reader does not know the study by Bergvall et al. (2007). Either this part of discussion should be deleted, or more information on the ‘mass-balance model’ (use different term? Note that Richards and CDE are also mass-balance equations) used in Bergvall et al. would be needed.

(6) Could you show simulated time series of concentrations and fluxes at the 10-m deep bottom of the vadose zone, serving as input to the GW model? Perhaps these can be compared to simulation results of the mass-balance model. Perhaps mean transit times are similar, but peak events differ. How could this affect overall transit times towards the extraction wells? Can you better demonstrate the benefit of using your coupled approach?

(7) Although using daily time steps may be a high time resolution for this long-term study, in terms of process time scale it is not. If daily averages are used, the rainfall rate will less often exceed Ksat (assuming measured value) of the soil than if real rates (e.g., hourly time steps) would be applied. Thus, saturation of soil layers is not reached or less often. The higher sensitivity to infiltration than to Ksat(soil), reflects this. So overall the ranking of sensitivities is meaningful only within the (time scale of) this modelling approach.

It seems that macropore flow effects were not required to explain the observations. Although calibrated large macrodispersivity values in the unsaturated zone point to non-ideal transport. The macropore flow discussion could be shortened (or skipped altogether).

The moving average procedure in Fig. 4 is unclear.

The contrasting concentration patterns in Fig. 5 for west and east wells could be explained better, e.g., by using graphical representations of the plume and velocity vectors in and between pumping periods.

Extra need for clarification is also suggested below in the specific comments. I suggest that this study can be published in HESS after revision.

SPECIFIC COMMENTS

ABSTRACT Line 4: In formerly glaciated areas – regions

Line 7: subsurface transport of pesticides in extensive glaciofluvial and littoral sediments – not soil?

Line 9: point scale – or soil profile scale.

1 INTRODUCTION

Page 1731, Line 4: As part of a national monitoring program, 28% of the groundwater supplies investigated between 2005 and 2008 were [add: identified as being] contaminated...

Page 1731, Line 11: “approximately one hundred groundwater supplies were recently closed due to BAM contamination” - what means “supplies” – extraction wells? Certainly not entire waterworks?

Page 1731, Page Line 15: “Dichlobenil has largely been used as a pesticide” – was mostly used as a herbicide

Page 1732, Line 15: “The lack of models for eskers . . .” define eskers, since this may not be known to all readers. I wonder if this statement is accurate: not most aquifers will be eskers even in regions that were glaciated during the last ice age – there are other types of glaciofluvial sediments that are widespread? So make statement more general?

2 MATERIALS AND METHODS 2.1 Modeling approach

Page 1733, Line 6: “. . .the calculated pesticide concentration from the vadose zone model was used as the input” – questions on the coupling: you would rather need both concentration in percolate and volume of water exchanged; so the mass flux. Please clarify. Other questions: coupling at what depth? Time resolution of one day? Was water flow also used as input to Modflow/MT3DMS via sink/source term? Maybe add ‘see below’ or the like, if these things are explained in a later section.

Page 1734, Line 8: “. . .theta is the porosity” – in eqs. 1 and 2 theta denotes water content. Use different symbols? Page 1734, Line 13: “To evaluate the robustness of the model’s predictions” – what means “the model” – eqs. (1) through (4) (Hydrus+Modflow+MT3DMS)?

Page 1734, Line 13: “were perturbed with changes of ± 2 to 10%, corresponding to the observed variability (Bergvall et al., 2007)” – is not this quite a small variability, thinking of, for example, infiltration into soil and hydraulic conductivity of soil or aquifer? Natural rainfall intensity and such parameters can vary much more. Please explain.

2.2 Field site description Page 1735, Line 24: “The former nursery is situated on well-sorted, unstructured, littoral sand and lenses” – what about the soil type and physical-chemical soil properties at this site? Soil properties have a strong effect of sorption and degradation.

2.3 Data sampling – unsaturated zone Page 1736, Line 9: “At one identified hotspot (Fig. 2)” – I could not locate this hotspot in Fig. 2, apply symbol and indicate in legend?.

2.4 Data sampling – saturated zone Page 1737, Line 13: “The mean leakage was estimated to be 5% of the mean discharge rate of 160 l s^{-1} (SMHI, 2009).” Does this 5% loss significantly exceed the error margin of the discharge rate measurement?

Page 1738, line 3: “Assuming a Gaussian distribution, the longitudinal dispersion ranged between 0.2m and 1.5 m, at the 2m scale.” Gaussian distribution (in horizontal direction!?): what assumption is underlying here – advection dispersion? But is 1.5 m dispersivity within 2 m transport distance not rather long for AD behaviour?

2.5 Application of modeling approach 2.5.1 Vadose zone model

Page 1738 – Line 6: “The decoupling of the vadose and groundwater zones was found to be appropriate since there was little variation in the groundwater table depth” – Decoupling - does this mean no GW recharge through the vadose zone was assumed? How does then the solute get into the GW model, is it just added as mass?

What (is the range in) surface area(s) that was (were) represented by the point-scale model? Was every grid cell of the subsurface model coupled with the 1 D model, or were the hydrologic units? Explicitly mention narrow grid spacing of 2 cm (which is sufficient resolution for valid calculation: Vogel, H.-J., Ippisch, O., 2008. Estimation of a Critical Spatial Discretization Limit for Solving Richards’ Equation at Large Scales. Vadose Zone J., 7(1): 112-114).

Page 1738 – Line 18: “Ten soils with various properties were defined to describe the vadose zone, ranging from fine sandy silt to coarse sandy medium sand (Table 3).” Add: “The information underlying Table 3 was obtained as follows”. Some measurements were already mentioned above, but it is not clear what information entered the table – including parameters for chemical reactions. The remainder of this page reads like a discussion of the validity of the data, but does not explain how they were derived, which I found confusing. Adding some explicit statements in this part would be helpful.

Page 1739, Line 1: “As moderate concentrations of dichlobenil were found at depths greater than 0.9 m, we assumed that the linear Freundlich sorption isotherm was applicable." To make immediately clear that linear isotherm was used only for the depth below 0.9 m, I suggest to restate "At depths greater than 0.9 m, moderate concentrations of dichlobenil were found, so we assumed that the linear sorption isotherm was applicable." However, I do not understand the proposed relation. Why should moderate concentrations point to a linear isotherm?

Page 1739, Line 5: "Dispersivity was initially assumed to be 10% of the soil-profile depth, but was calibrated to 5 m, except for the top meter which was calibrated to 1 m." Can you squeeze in dispersivity values (an important model parameter) into Table 3? Indicate a possible physical interpretation of these extremely large dispersivity values of up to 5 m?

Page 1739, Line 23: "The van Genuchten-Mualem parameters were calibrated against water content measured at 51 depths on 13 occasions. The mean error of the total water balance was 1.3%." If the water balance was known, why was this information not used in the model calibration to better constrain the model? Was the calibration for water and solute done sequentially (literature says its better to do it simultaneously to utilize mutual dependencies). And the statement does not tell if this calibration is for one point only, or for several sites – the profile hydraulic properties certainly show spatial variability?

Page 1739, Line 27: "The solute component of the model was calibrated to achieve the best match between the calculated and observed concentrations of dichlobenil and BAM, in the solid and solute phases." Fitting which parameters? Fitted at what place – an average of the 5 sampling locations at nursery area? If stated above, briefly repeat here for clarity. Perhaps refer to results from sensitivity analysis (some 'see below' statement) used to identify the important parameters to be fitted.

2.5.2 Groundwater model Page 1740, Line 8: "Initially, the groundwater table was calculated in a one-layer model with the same boundary conditions." What was the result

of using one layer and why was it discarded? If not important, delete statement.

Page 1740, Line 20: "Four different recharge rates were defined for the model: most areas had a constant net infiltration rate of $8.2\times10{-}4$ md-1." Does this number correspond to what is simulated with the 1 D model at 10.2 m depth? If there is a considerable difference, this affects the simulated loss of pesticide to the GW.

Page 1742, Line 1-3. "The simulation started on 1 January 1976 and the calibration model was run for 33.5 yr until 1 July 2009. The prediction model was run for 45 yr until 31 December 2020." – Was the vadose zone model also run for this time and if not, how was the coupling for times covering different simulation periods done?

Page 1742, Line 1-3. "Calibration of dispersivity in the three dimensions was conducted manually" – why, was there no automated calibration for solute transport available?

Page 1742, Line 18: "Equation (6) gives a longitudinal dispersivity of 0.96m at the grid-cell scale" if that is a correct application of Eq. 6 to use it for the grid cell size of 20 m (and not for the entire aquifer dimension), then what is it supposed to describe – numerical or physical dispersion?

Page 1742, Line 21: "...and sorption is limited." How does sorption reduce lateral dispersion (add reference?)

3 Results Page 1743, Line 13: "The saturated hydraulic conductivity " add: "of the aquifer"

Page 1743, Line 13: "Together with the infiltration rate" D'accord, but one should be aware that the sensitivity of infiltration rate and van Genuchten parameters certainly depend on the time resolution of the model simulation. Although using daily time steps may seem as a high time resolution for this long-term study, in terms of process time scale it is not. If daily averages are used, the rainfall rate will less often exceed the Ksat of the soil than if real rates (hourly time steps) would be applied. The higher sensitivity to infiltration, than to Ksat(soil), may reflect this. So overall the ranking of sensitivities is meaningful only within the (time scale of) this modelling approach.

Page 1743, Line 18: "The simulated and observed concentrations, at one observation well at the nursery and at the extraction wells, are shown in Figs. 4 and 5." – Please briefly explain moving average procedure in Figure 4

Page 1744, Line 13: "At the end of the predictive simulation," – in 2012?

Page 1744, Line 20: "The simulation of the vadose zone gave a median transit time" – what sample does the median refer to – averaged over number of years? Or the number of 1D models linked to the GW model – but there seems to be only a single model, i.e. uniform conditions from upper boundary (was there no spatial variability in infiltration in the contaminated area)? Was the vadose zone model(s) only used in the contaminated area (tree nursery), while outside of this area, the upper boundary condition of MODFLOW was equal to prescribed GW recharge or recharge related to some leakage and conductance? I do not recall this being explained somewhere. At least this info could be added in Fig. 3. Page 1745, Line 3: "and the simulation was run with pumping rates of 1.5 l $s-1$ and 0.75 l $s-1$." Why larger values in simulation than in test– explain.

4 Discussion It comes a bit as a surprise that the discussion starts with a comparison between this approach and another approach which was here for the first time.

Page 1745, Line 17 "However, in the vadose zone the models gave similar median transit times for both water and BAM." – To avoid possible confusion in this statement (transit time of water similar to that of BAM), consider adding "with similar retardation factor of 1.7." How is the transit time of the mass balance approach calculated?

Page 1746, Line 1: "We considered whether macropore flow should be included in the model. During our simulation time of 33.5 yr, the maximum infiltration rate was 40mmday-1. Compared to the saturated hydraulic conductivity at the soil surface, this is 1000 times smaller and indicates that matrix flow is the dominant process." Be

careful, daily averages cannot be compared to values for Ks measured under 'real-time conditions'. The main rainfall event on the day with 40 mm rainfall may have had an intensity of, e.g., 20 mm/h. OK, that is still much smaller than Ks at the surface, but in lower layers the situation is different.

Page 1746, Line 5: "The pressure heads were studied with our model, but they were not higher than -0.75m at any time-step or depth." – Again, that is caused by your choice of daily time steps, unless Ks values are somehow calibrated for exactly this time interval used in the boundary condition. Else if measured values are used, the conclusion is not correct. The next statement about coarse texture is a stronger argument against macropore flow, although other forms of preferential flow (fingering etc.) might still play a role.

Page 1746, Line 14: "apparently higher dispersion than the true dispersion." Which you are already doing, right, using macrodispersivity values in the m range.

I wonder why you are discussing macropore flow in the first place? Were there any hints at macropore flow? There is no feasible way to test it experimentally for a 10 m deep vadose zone. While flow in the vadose zone is almost never one hundred per cent chromatographic, I would assume from your description that this seems to be a relatively homogeneous flow case. This can indeed be represented by an increased macrodispersivity.

Page 1746, Line 24: "the integral of the observed concentrations" – integral over what giving what quantity; define this above, at first reference to Figure 4.

Page 1747, Line 6: "In this well, the concentration increases when the pumps are stopped because the contaminated water becomes less diluted (Fig. 5)." This will correspond to a shift in the flow direction to the natural one (after stopping pumping) favoring the west well, whereas the east well is partly (in Layer 2) outside the esker. Is that an explanation for the contrasting concentration patterns?

Page 1747, Line 26: “be clean in four years.” Means: c < 0.1 μg/L. 5 Conclusions

Page 1748, Line 8: “This paper describes a [a coupled vadose zone – Groundwater] model for pesticide transport” –

Page 1748, Line 11: “With the combination of a deep vadose zone and coarse texture, macropore flow was found to be of minor importance for contaminant transport.” – add that the observed concentrations could be described by the model without assuming macropores. Although a large macrodispersivity was calibrated suggesting deviation from chromatographic transport.

Comment: If macrodispersivity was required, why was the travel time equal to a simple mass balance approach? Furthermore, this approach was not explained with regard to the treatment of surface applied pesticides and how they get to GW).

Page 1748, Line 21: “Further development of the model would require additional field measurements to assess the importance of macropore flow in deep, sandy aquifers. It is also important to characterize the variability of hydraulic conductivity and its effect on contaminant transport in eskers.” Statement 1 is conflicting with what is previously ysaid, namely, that macropore flow does not play a role in deep vadose zones. Statement 2 is not convincing either; what deficiencies in the present study can serve as an argument for studying this?

Tables

Table 1: averages for samples taken from 5 locations and depths up to 7 m ? 10 m? I would not use logarithm of K slug test, but the original values, which is consistent with other K units in the rest of the paper.

Table 2 with Figure: It is unsual to include a Figure in a Table. The Figure should be stand-alone and larger.

Table 3: Indicate in Table 1 (e.g., using superscript symbols) which quantities were measured, which calibrated, and which represent literature estimates. Add dispersivi-

ties to Table 1.

Table 4: obtained for what time frame of simulation?

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