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Exploring an aquifer system by integrating hydraulic, hydrogeologic and environmental tracer data in a three-dimensional hydrodynamic transport model

N. Mattle[a,b], W. Kinzelbach[b], U. Beyerle[c,d,*], P. Huggenberger[e], H.H. Loosli[a]

[a]*Physics Institute, University of Bern, CH-3012 Bern, Switzerland*
[b]*Institute for Hydromechanics and Water Resources Management, ETH, CH-8093 Zürich, Switzerland*
[c]*Department of Water Resources and Drinking Water, Swiss Federal Institute of Environmental Science and Technology, EAWAG, CH-8600 Dübendorf, Switzerland*
[d]*Isotope Geology, Swiss Federal Institute of Technology, ETH, CH-8092 Zürich, Switzerland*
[e]*Institute of Geology and Paleontology, University of Basel, CH-4056 Basel, Switzerland*

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Abstract

This article presents a numerical model of a part of an aquifer that is recharged by infiltration from the Swiss pre-Alpine river Töss in the Linsental (north-eastern Switzerland). The nearby city of Winterthur makes use of this aquifer as a resource of drinking water. The presented model is part of a larger interdisciplinary research program undertaken with the goal to evaluate the possible impacts of a planned revitalization of the severely canalized river Töss. Above all it should show the extent of decrease of the groundwater residence time if the river bed is allowed to move towards the drinking water wells.

The flow model was constrained and calibrated by transport modelling of tritiogenic ^{3}He. This tracer reflects both the aging of the water (by accumulation of ^{3}He resulting from tritium-decay) as well as the two different components of the mixture (river water free of tritiogenic ^{3}He due to degassing, and groundwater enriched in ^{3}He due to accumulation). By simulating a Dirac-pulse-shaped input of a conservative tracer at different sources (river cells or upstream flux boundary cells) it is possible to determine the age distributions as well as the mixing ratios of the two types of water at the two pumping stations within the model area. The same calculations for a hypothetical river course passing directly beside the pumping stations indicate a decrease of the mean residence time of the pumped water together with an increase of the amount of the younger river water component. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Groundwater; River/groundwater interaction; Sedimentological model; Model calibration; Predictive modelling; Environmental tracers; Tritiogenic ^{3}He

1. Introduction

In Alpine and pre-Alpine countries like Switzerland, young groundwater is commonly used as drinking water. A remarkable amount of this groundwater is recharged by infiltration of river water. For the protection of these groundwater resources, the information about the mean residence time and the

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* Corresponding author. Department of Water Resources and Drinking Water, Swiss Federal Institute of Environmental Science and Technology, EAWAG, CH-8600 Dübendorf, Switzerland. Tel.: +41-1-823-55-33; fax: +41-1-823-52-10.

E-mail address: beyerle@eawag.ch (U. Beyerle).

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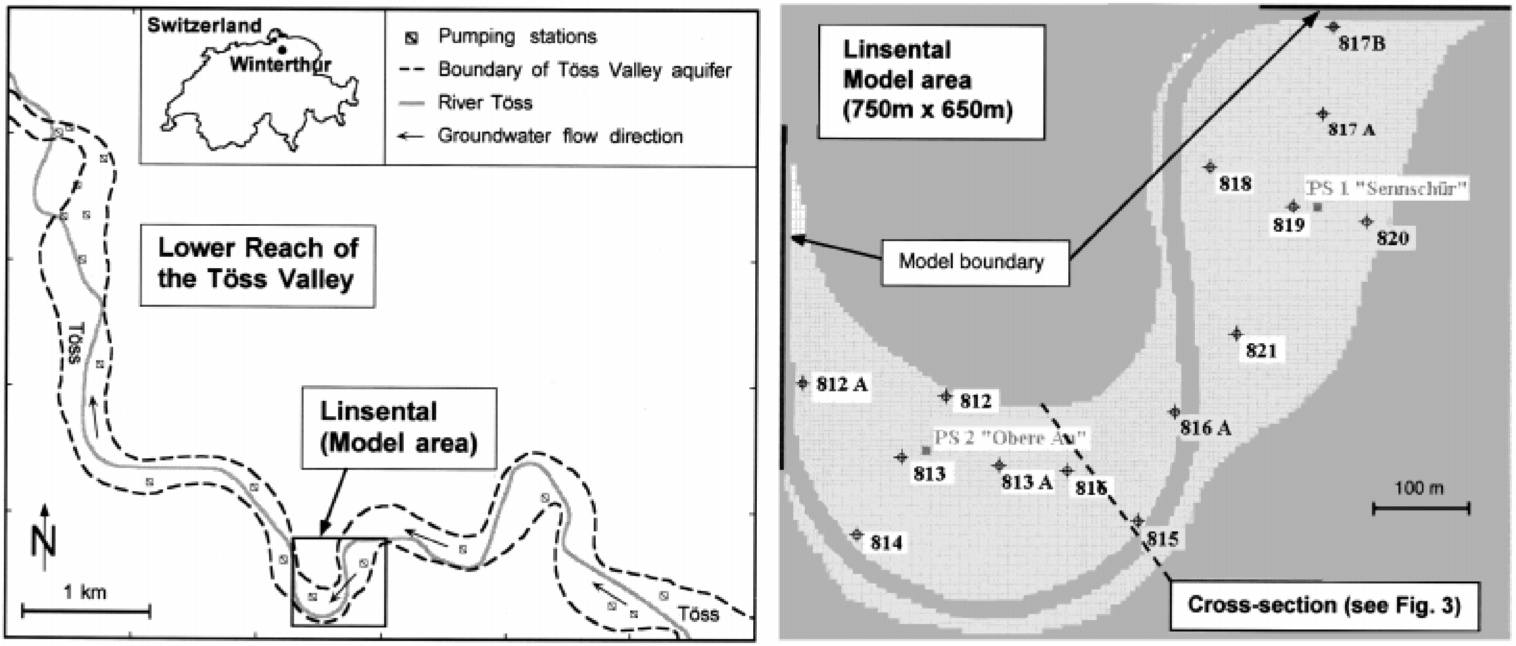

Fig. 1. Geographic situation of the Linsental, a part of the Töss Valley south to the city of Winterthur, Switzerland. The map on the right shows the location of the cored boreholes (numbered 8xx and 8xx A) and the two pumping stations within the model area.

dynamics of water exchange between river and aquifer is of central importance. A way to derive such information is the integration of hydraulic, hydrogeologic and environmental tracer data in a comprehensive flow and transport model.

The work is performed in the following steps:

- a conceptual sedimentological model of the aquifer was constructed on the basis of geophysical and stratigraphic borehole data;
- the flow model parameters were constrained by pumping test data and calibration;
- environmental tracer transport was modelled and the results were subject to a sensitivity analysis;
- the leakance of the river bed, which turned out to be the critical parameter, was recalibrated using the observed tracer concentrations in the wells;
- finally, predictive modelling for a different river flow regime was performed.

2. Description of the model area

The Linsental is a small section of the Töss valley south of the city of Winterthur in the canton of Zurich, Switzerland (see Fig. 1). It originated from fluviatile erosion of the Upper Fresh Water Molasse (Kempf et al., 1986) followed by infill of coarse fluvial gravels, overbank- and flood deposits. These deposits form an aquifer which is fed mainly by the infiltration of river water. The shallow aquifer in the Linsental has a maximum thickness of 25 m and an average width of 200 m (Fig. 1). The aquifer is highly heterogeneous as depicted by hydraulic conductivity values ranging from 10^{-2} m/s (highly permeable gravels) to 10^{-5} m/s (clay lenses).

The city of Winterthur makes use of this aquifer as a resource of drinking water. Within the model area extending over 650×750 m^2, there are two pumping stations (PS1 called “Sennschür” and PS2 called “Obere Au” in Fig. 1). The depths of the filters of the wells are 10 m (“Obere Au”) and 12 m (“Sennschür”) below the river bed, respectively. They are designed as horizontal filters with a length of about 10 m.

The infiltration of river water seems to be subject to seasonal variations as can be concluded from ^{3}H/^{3}He investigations in the model area (Beyerle et al., 1999). The samples from shallow boreholes showed a distinct variation of water age over time. The observed decrease of mean water age in summer indicates that locally infiltrated river water dominates the shallow part of the aquifer whereas in winter the local infiltration is reduced thus leading to an increase of the mean residence time found in the shallow boreholes. This fact can be explained by heavy rain and flooding events occurring frequently in summer. However, for the samples from the deep boreholes an almost constant ^{3}H/^{3}He water age was observed over time. Therefore in the deep part of the aquifer (involving the two pumping stations) the tracer distribution can be considered to be in steady state (Beyerle et al., 1999).

The Linsental was chosen by the local water authority to investigate into the possibilities of a revitalization of the severely canalized river Töss. This leads to a conflict of interests with the water supply who fear that the water quality of the wells deteriorates as a consequence of the river bed moving towards the drinking water wells. A changed flow regime could decrease the residence time of the water in the aquifer thus increasing hygienic risk. Therefore various hydrological and hydrogeological investigations were recently undertaken in the Linsental providing a good database for the development of a numerical flow model. Within the model area 14 cored boreholes exist which were analysed with respect to their lithological structure as well as their hydraulic conductivities.

3. Description of the model parameters and flow model results

The steady-state flow equation of an aquifer is given by

$$\nabla(\mathbf{K}\cdot\nabla h) + q = 0$$

where h is the piezometric head (m), $\mathbf{K}$ the tensor of hydraulic conductivity (m/s) and q the recharge/discharge rate per unit volume (s^{-1}).

In addition boundary and initial conditions are required. The acquisition of model input data is described below.

The lower boundary of the aquifer is defined by the

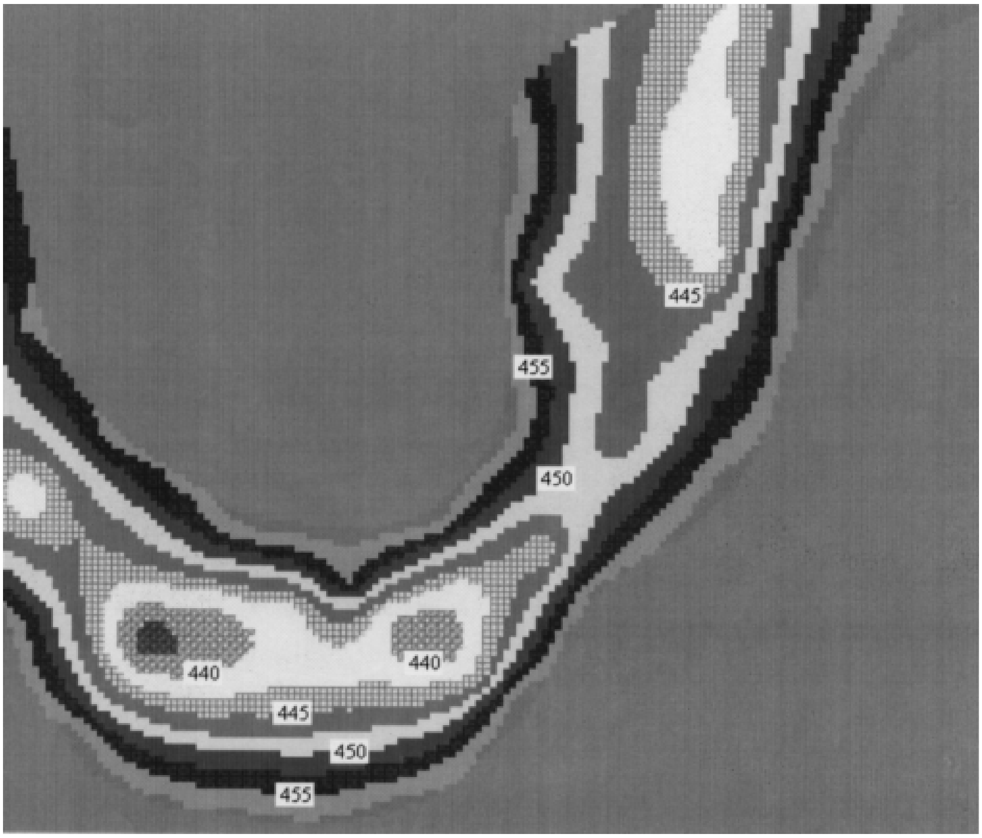

Fig. 2. Topography of the lower boundary of the aquifer interpolated from the top levels of the Molasse layer observed in the boreholes. The numbers represent the elevation of the contour lines in m amsl. The maximum thickness of the aquifer amounts to 20–25 m.

Molasse bedrock consisting of impervious sandstone and marl. The corresponding hydraulic conductivities are lower than 10^{-6} m/s. The topography of the bottom of the aquifer was interpolated from the top levels of the Molasse layer observed in the boreholes (Fig. 2). In the aquifer channel one can see an elevated Molasse saddle in the middle of the model area, which separates two deeper sections of the aquifer containing the drinking water wells.

For the distribution of the hydraulic conductivity of the underground, a sedimentological approach was chosen which takes into account the genesis of the aquifer. On the basis of historical documents, core descriptions and ground-penetrating radar (GPR) measurements, which allow one to identify geological units from spatial variations of high-frequency electrical properties (for gravels mainly due to varying water-content), one can assume that in the past the course of the river Töss mainly occurred in two different modes. In the first mode the river bed followed today's course, in the second it followed a course along the opposite side of the valley. The formerly active river channels are mainly filled by gravels and sands without any clay, resulting in a high hydraulic conductivity. The former flood plains beside the active channels consist of fine-grained overbank deposits (silty-sand) and of coarse gravel sheets with major amounts of fines (silt and clay) deposited during major floods; the resulting loam is characterized by a relatively low hydraulic conductivity. The temporal sequence of the different modes can be derived from the cross-section which was constructed on the basis of the sedimentological analysis of cores and the GPR investigations (Fig. 3). Corresponding to this sedimentological conceptual model the flow model is parametrized

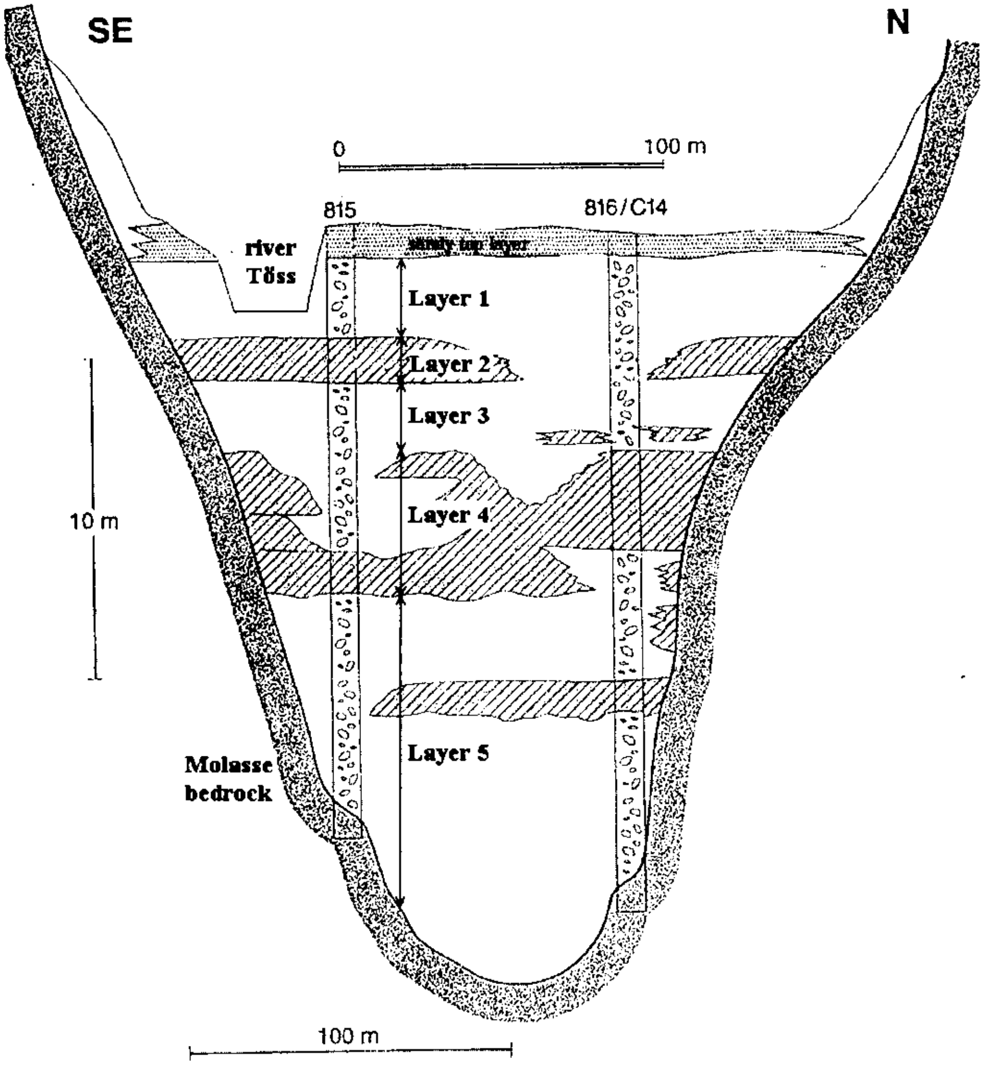

Fig. 3. Cross-section through the Linsental aquifer constructed on the basis of cored boreholes and ground-penetrating radar (GPR) investigations. The well developed, formerly active river channels together with some transition layers form the more permeable sections of the aquifer while the hatched areas represent the former floodplains with low conductivity. To implement the sedimentological conceptual model in the three-dimensional flow model at least five layers were necessary to resolve the most important features in the vertical extension of the aquifer.

by two horizontal hydraulic conductivity values only. The corresponding vertical hydraulic conductivities were chosen an order of magnitude smaller than the horizontal conductivities because of the sedimentary nature of the alluvial aquifer (e.g. Bouwer, 1978). The sedimentological approach allows the reduction of the number of degrees of freedom of the model substantially. This is necessary, as the possibilities for the determination of distributed parameters in a 3D model by calibration are very limited.

Hydraulically, the Linsental aquifer is dominated by abstraction of groundwater from the two pumping stations and by infiltration from the river Töss. Direct groundwater recharge by precipitation can be neglected against the infiltration of river water. The groundwater recharge by infiltration from the river Töss is controlled by the piezometric heads of the

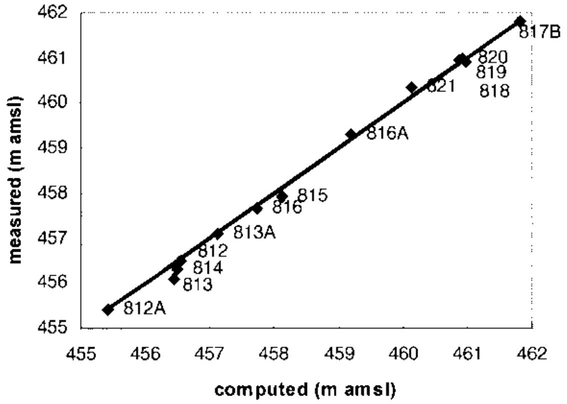

Fig. 4. Comparison of measured and computed piezometric heads of 13 boreholes within the model area after steady-state calibration. The estimated parameters include the conductance of the river bed as well as the hydraulic conductivities.

aquifer, the river water levels along the river course and the hydraulic conductance of the river bed. The latter depends strongly on the state of clogging of the riverbed and can vary in space and time. In order to maintain a limited number of degrees of freedom of the model the variation of the hydraulic conductivity in space and time could not be taken into account.

The choice of the upstream and downstream model boundary was inspired by the course of the river (see right part of Fig. 1). Fixed head boundaries reflect a good approach to the natural circumstances because of the good hydraulic connection between the river and the aquifer. Note that the groundwater in the model consists of a mixture of water infiltrated from the river within the model area and water entering the model domain from the upstream part of the aquifer.

The values for the hydraulic conductance of the river bed and the hydraulic conductivities of the two types of aquifer material introduced were estimated by steady-state calibration using the 3D code MODFLOW (McDonald and Harbaugh, 1988) in combination with the pre- and postprocessor PMWIN (Chiang and Kinzelbach, 1996). No unique solution was found. However, good fits were obtained for values centred around 3×10^{-4} m^2/s for the conductance of the river bed, 2×10^{-3} m/s for the higher and 2×10^{-5} m/s for the lower horizontal hydraulic conductivities (Fig. 4).

After having provided the necessary model parameters the steady-state flow conditions can be calculated. The three-dimensional streamlines are shown in Fig. 5 as horizontal projections on the top and as vertical projections on the frontal and lateral sides of the modelled volume. One can see that both wells extract deeper groundwater entering the modelled domain through the upstream model boundary as well as river water infiltrated in the vicinity of the wells. Infiltration of river water occurs all along the river and exceeds exfiltration of ground water into the river that takes place mainly along the downstream model boundary. The Molasse saddle forces the deeper ground water of the upper river loop to rise to upper layers and enhances the mixing with the river infiltrate of the same loop because of the higher heterogeneity of those layers. Groundwater that is not captured by the wells takes about one year to travel through the whole model area. The spectrum of residence times for the abstracted river water as well as the mixing ratios between local river infiltrate and older groundwater can be analysed by transport modelling (see Section 5).

4. Results of the transport modelling of $^3He_{tri}$

Based on the flow model, tracer transport was calculated with MT3D using the finite difference method (Zhen, 1990). For the investigation of river–groundwater interaction tritiogenic helium ($^3He_{tri}$) originating from the decay of tritium (^3H) proved to be a valuable tracer (tritium half-life: 12.38 year; Oliver et al., 1987). On one hand it is sensitive to the mixing ratio between $^3He_{tri}$-free river water and $^3He_{tri}$-enriched older groundwater, on the other hand the extent of $^3He_{tri}$-accumulation in groundwater depends on the residence time. Because of this ambiguity there is no unique interpretation of an observed ^3He-value. The residence time, however, is mainly given by the distribution of the hydraulic conductivity based on the conceptual sedimentological model of the aquifer. Therefore successful modelling of tritiogenic ^3He only confirms the mixing ratios between river water and groundwater.

Transport modelling requires a few more model parameters than flow modelling such as effective porosity, dispersivities, decay or degradation rate and adsorption parameters of the tracer. A value of 0.25 for the effective porosity is considered

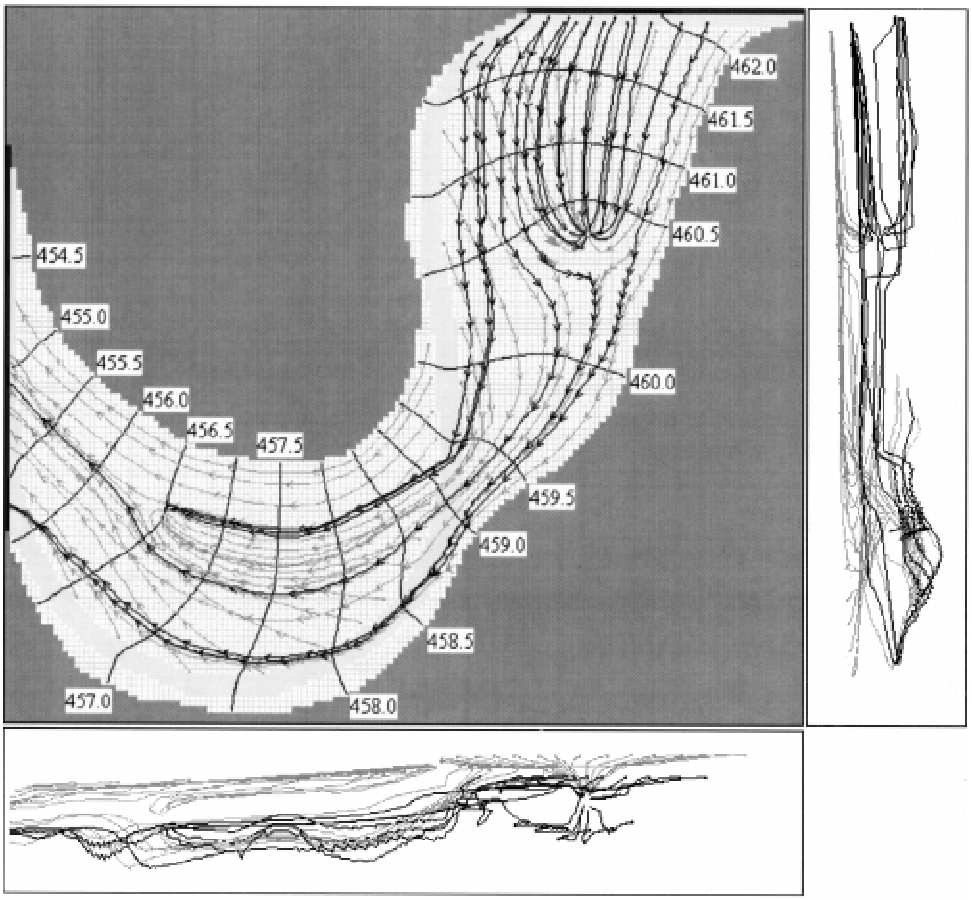

Fig. 5. Streamlines for steady-state conditions shown as horizontal projections on the top and as vertical projections on the frontal and lateral sides of the modelled volume. The numbered black lines represent the isolines of the water table elevation in the top layer of the aquifer (m amsl). Streamlines are entering the aquifer from the river cells of the upper and the lower river loop (grey lines) and from the 'fixed head' cells of the upstream model boundary (black lines). Neighbouring arrows on the streamlines mark a travel time interval of ten days.

reasonable for the Töss valley. The longitudinal dispersivity was estimated from the scale length of the transport phenomenon. Its scale dependence has been observed for field-scale physical transport processes in many tracer experiments (Gelhar et al., 1992). For transport over distances between 100 and 1000 m the longitudinal dispersivity is roughly an order of magnitude smaller than the transport distance. Values of 20 m for the longitudinal dispersivity and of 2 m for both the horizontal and the vertical transverse dispersivities are reasonable values for the present transport model. The horizontal and vertical dispersivity values are not very sensitive as the gradients of concentration are small and a steady state situation is considered.

As a noble gas, ^{3}He does not undergo degradation nor significant retardation caused by adsorption. However, the ingrowth of ^{3}He by decay of tritium must be taken into account. MT3D supports irreversible reactions of the first order such as radioactive decay but not the ingrowth of a species by decay of its mother isotope. Therefore the accumulation of $^{3}\mathrm{He}_{\mathrm{tri}}$ had to be calculated as the difference between the modelled concentrations of ^{3}H as a conservative tracer and the modelled concentrations of ^{3}H taking into account the decay. This solution is satisfactory, as

Table 1
Upstream boundary concentrations of ^{3}H and ^{3}He$_{tri}$

	Depth (m below surface)	^{3}H (TU)[a]	^{3}He$_{tri}$ (cm^{3}STP/g)
Töss	–	27.0	0
Layer 1	0–5	27.0	1.0×10^{-15}
Layer 2	5–7	27.0	1.0×10^{-15}
Layer 3	7–9	25.7	3.5×10^{-15}
Layer 4	9–13	24.9	6.0×10^{-15}
Layer 5	13–ca. 25	24.0	8.4×10^{-15}

[a] 1 TU corresponds to a ^{3}H/^{1}H ratio of 10^{-18} and decays to 2.488×10^{-15} cm^{3}STP(^{3}He) g^{-1}.

the involved species do not differ in their characteristic transport parameters.

The boundary conditions for ^{3}H and ^{3}He$_{tri}$ were defined considering the observed concentrations in the river Töss and in the boreholes next to the upstream model boundary (see Table 1). Obviously these boundary concentrations have a stronger effect on the modelled concentrations for the nearby well "Sennschür" than for well "Obere Au" further downstream. The boundary concentrations in combination with the fixed head boundaries of the flow model result in a constant inflow of tracer through the upstream boundary of the model.

The result of the transport model is a spatial distribution of tracer concentrations. Fig. 6a shows the distribution of ^{3}He$_{tri}$ originating from tritium decay within the model area, while Fig. 6b shows the total ^{3}He$_{tri}$ including the amount imported via the upstream model boundary. A comparison of the two figures shows that ^{3}H-decay within the model area adds only a small amount to the total ^{3}He-concentration in the upper river loop; in the lower loop, however, its contribution amounts to up to 40%.

Comparing the calculated ^{3}He$_{tri}$-concentrations of the two wells with the measured concentrations (Table 2), one obtains a good correspondence for well PS1 "Sennschür". The computed value for well PS2 "Obere Au" is, however, about 40% lower than the observed value. Possible reasons could be:

- the well obtains more ^{3}He$_{tri}$-free river water in the model as a result of an overestimated value for the hydraulic conductance of the river bed;
- the ^{3}He$_{tri}$-rich deeper groundwater is too strongly diluted with river infiltrate in the model due to too high lateral dispersion coefficients;
- the flow velocities of the groundwater are too high (i.e. especially porosity may be underestimated), leading to a too low accumulation of ^{3}He$_{tri}$ by ^{3}H-decay.

A sensitivity analysis of the corresponding parameters shows, that the calculated concentrations mainly react to changes in the hydraulic conductance of the riverbed. The other parameters (effective porosity and lateral dispersivity) would have to be varied to unrealistic values to achieve the same effect.

5. Spectrum of residence times and mixing ratios of the well waters

Transport modelling offers a simple method to determine the residence times of the groundwater within the model area and the mixing ratios between river infiltrate and deeper groundwater in the wells. For that purpose, the transport of a conservative tracer is modelled which is introduced in the form of a Dirac-pulse applied to the inflows of the aquifer, namely the river and the upstream model boundary in our case. Under the assumption of small transverse mixing the normalized break-through curves (i.e. integral = 1) at the wells correspond to the spectrum of residence times. If the procedure is performed separately for the two types of inflow, the integrals over the respective break through curves allow the determination of the mixing ratios in the wells.

Comparing the normalized break-through curves calculated by transport modelling with the spectrum of residence times of a dispersion model, as it is often used for the interpretation of environmental radioisotopes (see e.g. Zuber, 1986), one gets good correspondence for the river water component in the well "Sennschür" (Fig. 7a). For well "Obere Au", however, a mixture of two components originating from different river sections and therefore with different mean residence times can be found (Fig. 7b). Depending on the mixing ratio a more or less well pronounced bimodal distribution of residence times develops that could only be reproduced ad hoc by two dispersion models in parallel respecting the exact mixing ratios (see below). This shows the advantage of the spatially

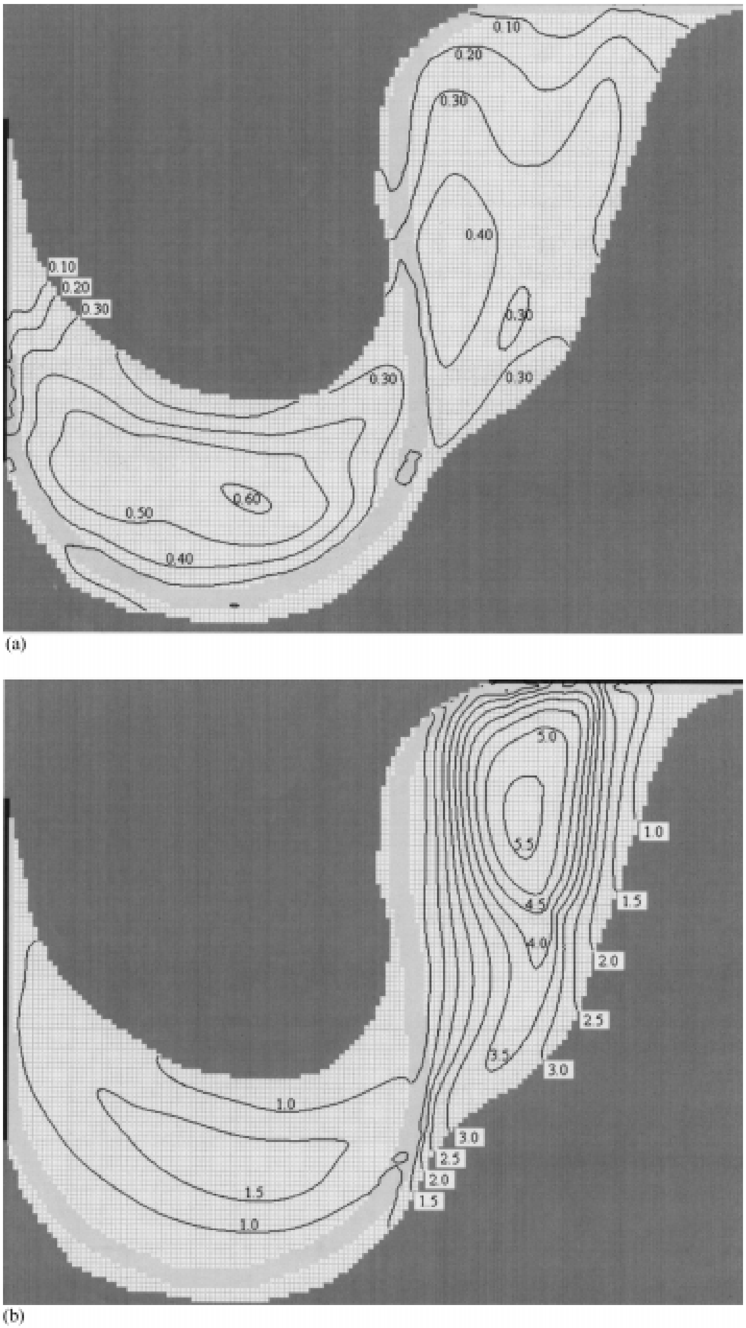

Fig. 6. Distribution of $^3He_{tri}$-concentration in the top layer of the aquifer: (a) tritium decay within the model area only; (b) tritium decay plus the amount imported via the upstream model boundary. The black lines represent the isolines of concentration in 10^{-15} cm^3STP/g.

Table 2
Measured and computed concentrations of tritiogenic ^{3}He (^{3}He$_{tri}$) for the two wells “Sennschür” and “Obere Au” for two different values of the river bed conductance

Pumping station	^{3}He$_{tri}$ computed conductance $= 3 \times 10^{-4}$ m^2/s (cm^{3}STP/g)	^{3}He$_{tri}$ computed conductance $= 1 \times 10^{-4}$ m^2/s (cm^{3}STP/g)	^{3}He$_{tri}$ “measured”[a] (cm^{3}STP/g)
“Sennschür”	5.08×10^{-15}	5.46×10^{-15}	$(5.1 \pm 1.0) \times 10^{-15}$
“Obere Au”	1.60×10^{-15}	2.27×10^{-15}	$(3.0 \pm 0.9) \times 10^{-15}$

[a] Calculated from the measured ^{3}He concentration according to Beyerle et al., 1999; error $= 1\sigma$.

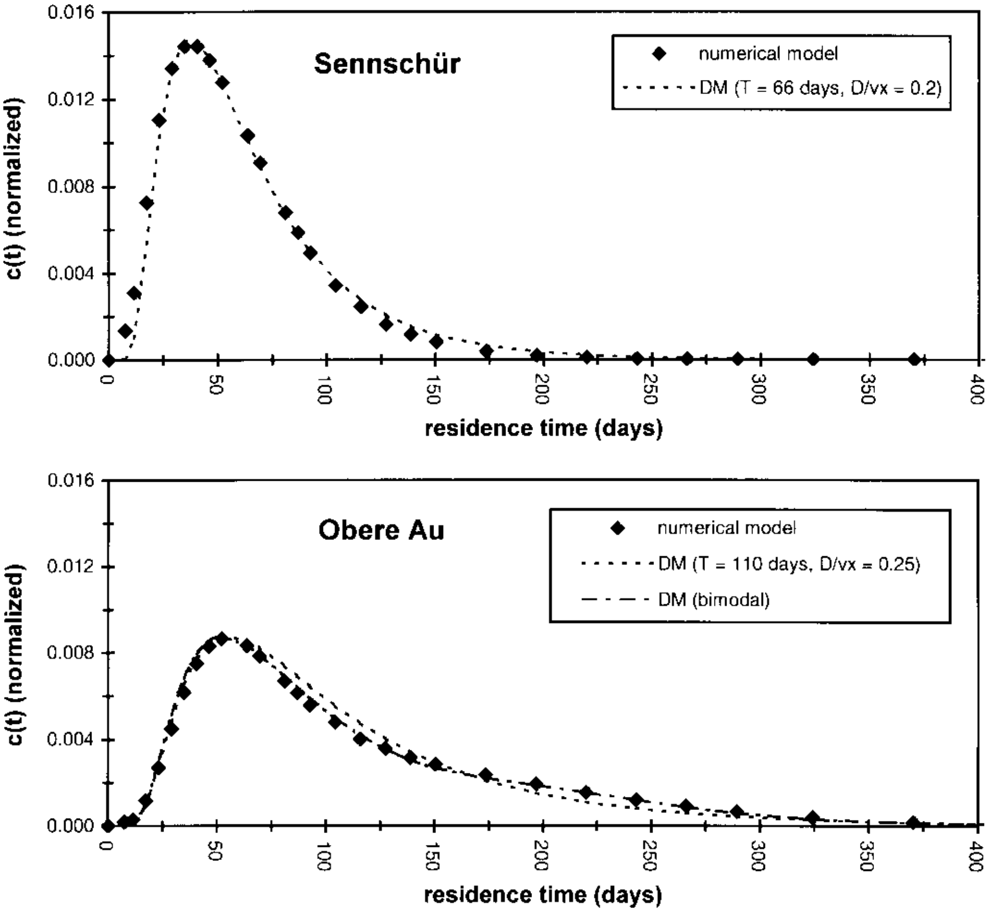

Fig. 7. Normalized (i.e. integral = 1) break-through curves of a conservative tracer computed for well “Sennschür” (a) and well “Obere Au” (b) as response to a Dirac-pulse injected to river cells (diamonds). The computed curves can be compared with the spectrum of residence times (dotted line) of a two-parameter dispersion model (mean residence time T and dispersion parameter D/vx). Because of the mixture of river water components with different mean residence times the computed break through curve at well “Obere Au” (b) cannot be reproduced by a simple box model. The resulting bimodal distribution of residence times (dashed-dotted line) could only be reproduced by two dispersion models ($T_1 = 100$ days, $D/vx = 0.23$ and $T_2 = 230$ days, $D/vx = 0.03$) in parallel respecting the exact mixing ratios ($N_1 = 90\%$, $N_2 = 10\%$).

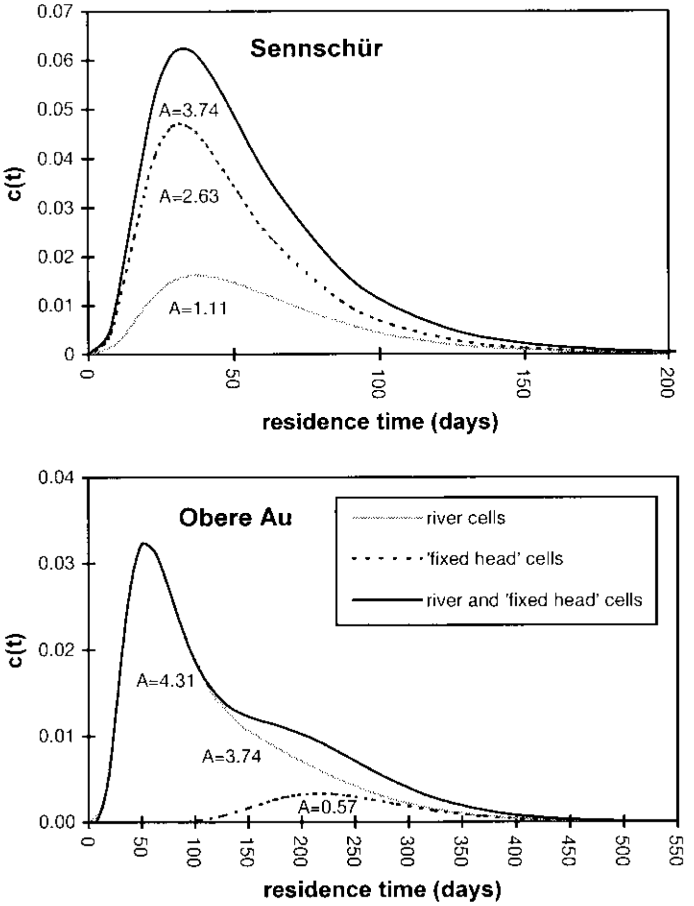

Fig. 8. Non-normalized break-through curves of a conservative tracer computed for wells "Sennschür" and "Obere Au" as response to a Dirac-pulse input to different inflows to the aquifer. The area (A) below the curves is equivalent to the amount of tracer being recovered by the wells from the different inflow sources and is used to obtain the mixing ratios in the wells (see text).

resolving model over a box model. In a box model a spectrum of residence times is assumed and its parameters are adjusted a posteriori. In the spatially resolving model the shape of the residence time distribution is a computed quantity. Fitting a box model to the situation would also require a time series of concentrations which is not available in the case described here.

The contribution of locally infiltrated river water calculated by means of the non-normalized break-through curves (Fig. 8) is higher for well "Obere Au" (87%) than for well "Sennschür" (30%), as was already expected on the basis of the general flow pattern. However, the comparison of the measured concentrations of $^{3}He_{tri}$ in the two wells shows that the share of river water in well "Obere Au" is overestimated by the model as a result of a too high assumed value of the hydraulic conductance of the river bed. The calibration of the flow model on the basis of heads is not sensitive enough to yield a unique value for this quantity. The concentrations of $^{3}He_{tri}$ in the wells on the other hand allow a sensitive calibration of the river leakance. With a conductance decreased by a factor of 3, the measured concentration of $^{3}He_{tri}$ in well "Obere Au" corresponding to a proportion of river water of 50–60% is reproduced by the model without deteriorating the calibration of the flow model (see Table 2).

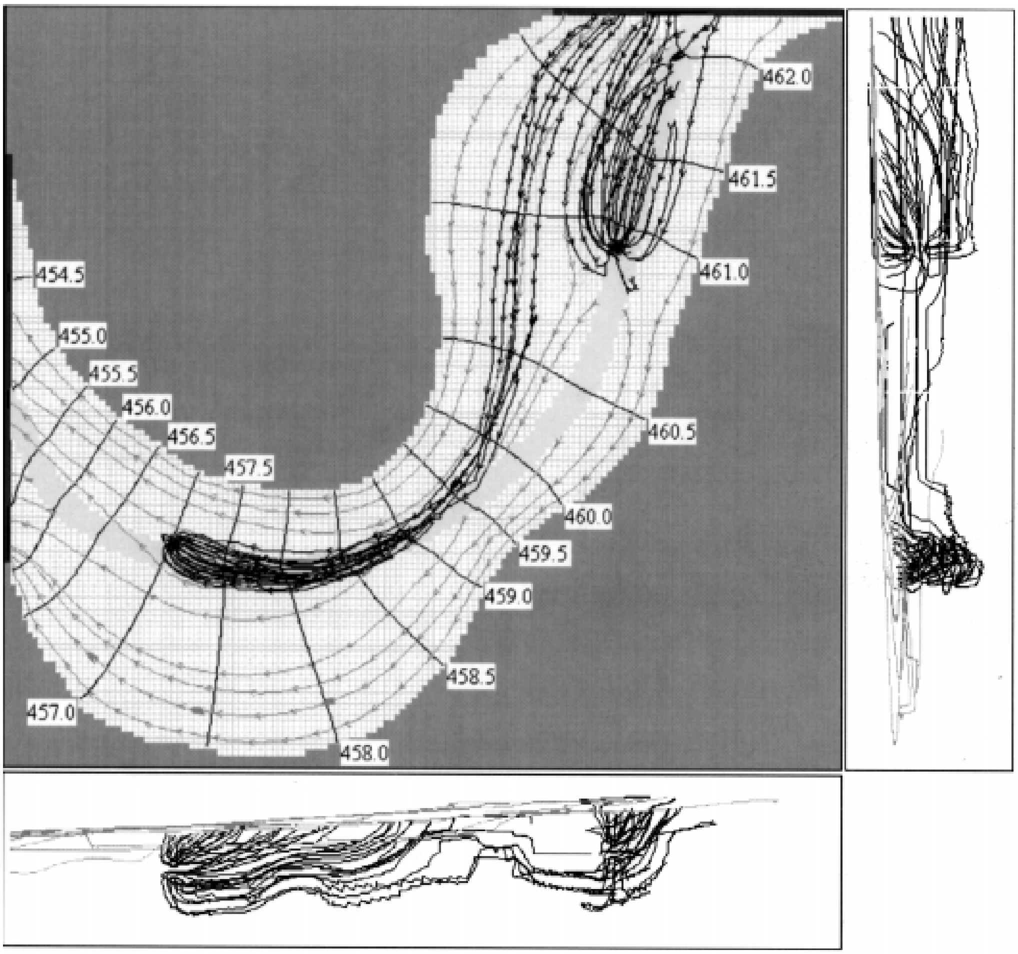

Fig. 9. Streamlines for steady-state conditions for a possible course of the river after revitalization (‘worst case’), shown as horizontal projections on the top and vertical projections on the frontal and lateral sides of the modelled volume. The numbered black lines represent the isolines of the water table elevation in the top layer of the aquifer (m amsl). Streamlines represent the flow patterns near the groundwater surface (grey lines) and the catchment areas of well “Sennschür” and well “Obere Au”, respectively (back lines). Neighbouring arrows on the streamlines mark a travel time interval of ten days.

6. Changes in flowfield, residence times and mixing ratios for a relocated riverbed

One advantage of a spatially distributed numerical model consists of the possibility to calculate different scenarios and to predict their effects. In our case, the flow conditions after a revitalization of the canalized river can be computed assuming that the conductance of the riverbed remains unchanged. In the worst case scenario the river Töss would choose its new riverbed close to the abstraction wells for the drinking water supply. Fig. 9 shows that compared to the flow conditions of today (Fig. 5) the catchment areas of the wells would be reduced with the consequence of narrower distributions of the residence times. On the basis of the newly calculated break-through curves a shift to smaller residence times has to be expected for the river water component of both wells, as well as an increase of the amount of river water especially for well “Sennschür”. This fact is also reflected by the shift of the cumulated age distributions of the pumped water to smaller residence times in

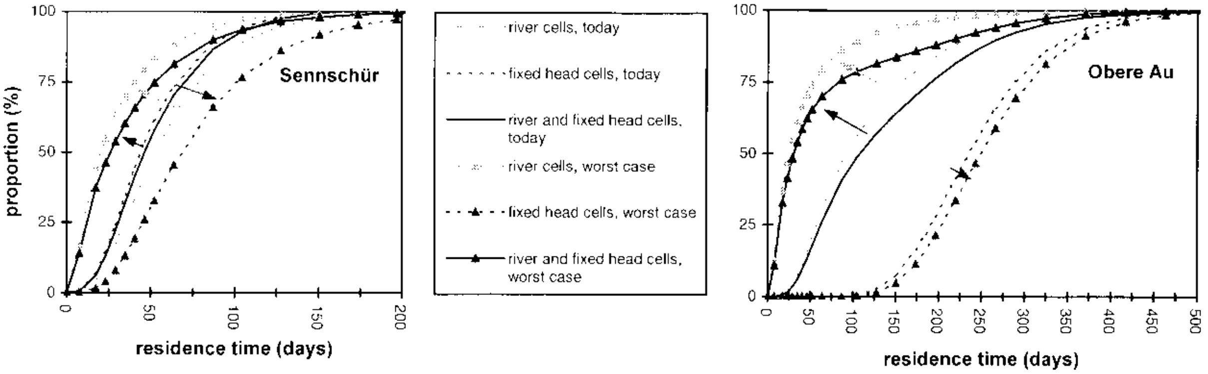

Fig. 10. Cumulated age distributions for the pumped water of the two abstraction wells. Curves without triangles, age distributions of the two different types of water of todays' state; curves with triangles, age distributions after revitalization (worst case scenario).

both abstraction wells (solid lines in Fig. 10). In contrast, the residence time of the pumped water component entering the modelled domain from the fixed head cells (dark dotted lines in Fig. 10) is slightly increased. This effect can be explained by a smaller hydraulic gradient between the upstream model boundary and the wells (compare Fig. 5 with Fig. 9). However, since the residence time of water originating from the river is decreased and at the same time its amount is increased, this effect is more than compensated.

7. Conclusions

The flow model presented in this study is based on a conceptual sedimentological model that allows significant reduction in the number of free model parameters. However, the gain in robustness of the model by reducing the number of free parameters is paid for by a loss of local quality of fit because the conceptual sedimentological model only represents the major structure and cannot reproduce local properties of the aquifer.

Transport modelling of tritiogenic ^{3}He clearly showed that the most important parameter for the river–groundwater system is the conductance of the riverbed. While the calibration of the flow model on the basis of heads did not yield a unique estimate of this parameter the transport model allowed to tune it much more sensitively.

One of the aims of this study was to predict the changes in the mean residence times of the drinking water wells as a consequence of a change in the river flow pattern. However, due to the high sensitivity of the conductance it is unrealistic to expect accurate predictions about changes in water quality due to the revitalization of the river. Yet, in the sense of a risk assessment the model predicts considerably reduced residence times and increased amounts of admixed river water if the riverbed moves close to the wells.

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