Calibration of a 3-dimensional Hydrodynamic Transport Model with Tritiogenic ^{3}He data

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Abstract

Simple box models such as exponential or dispersion models are a convenient tool in dating groundwaters on the basis of environmental tracer data. However, under certain circumstances (very young groundwaters, mixing of water compounds of different ages and origin, transient flow fields) these simplistic models lead to misinterpretation and the use of more complex and physical models such as 3-dimensional hydrodynamical transport models is appropriate.

This article presents a high resolution numerical mode1 of a part of an aquifer that is recharged by infiltration from the river Toss in the Linsental (north-eastern Switzerland). The flow mode1 was constrained and calibrated by transport modelling of tritiogenic “He. This tracer proved to be a good choice since it reflects both the aging of the water (by accumulation of “He resulting from tritium-decay) as well as the two different components of the mixture (river water free of ^{3}He due to degassing, and groundwater enriched in ^{3}He due to accumulation). By simulating a &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.

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

The present model is part of a larger interdisciplinary research program undertaken with the goal to evaluate the possible impacts of a planned revitalisation of the Swiss pre-alpine river Toss. 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.

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- 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.

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 [1] 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. This shallow aquifer has a maximum thickness of 25 m and an average width of 200 m. 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 m x 750 m, there are two pumping stations (PS1 called „Sennschür" and PS2 called „Obere Au" in Fig. 1).

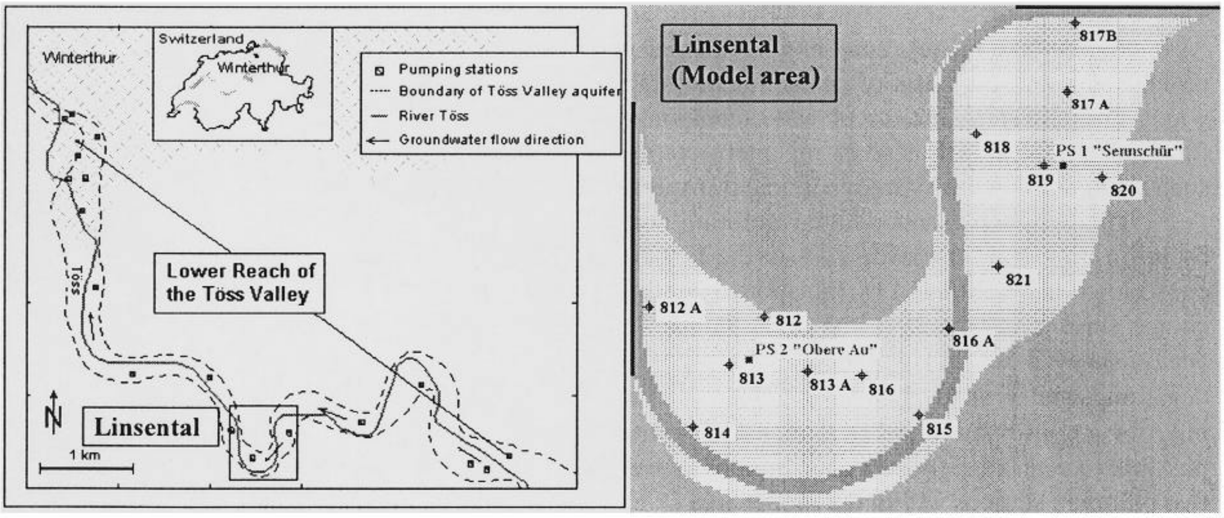


Fig. 1: Geographic situation of the Linsental, a part of the Töss Valley south to the city of Winterthur, Switzerland. The map on the right shows the location of the cored boreholes (numbered 8xx and 8xx A) and the two pumping stations within the model area.

3. Description of the Model Parameters

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

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

where

h is the piezometric head (m),

K is the tensor of hydraulic conductivity (m/s) and

q is the recharge/discharge rate per unit volume (s^{-1}).

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

The lower boundary of the aquifer is defined by the impervious Molasse bedrock. 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. Corresponding to this sedimentological conceptual model the flow model is parametrized by two hydraulic conductivity values only: one value for gravels in river channels and one for fine-grained overbank deposits. 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. [2]). The sedimentological approach allows to reduce 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.

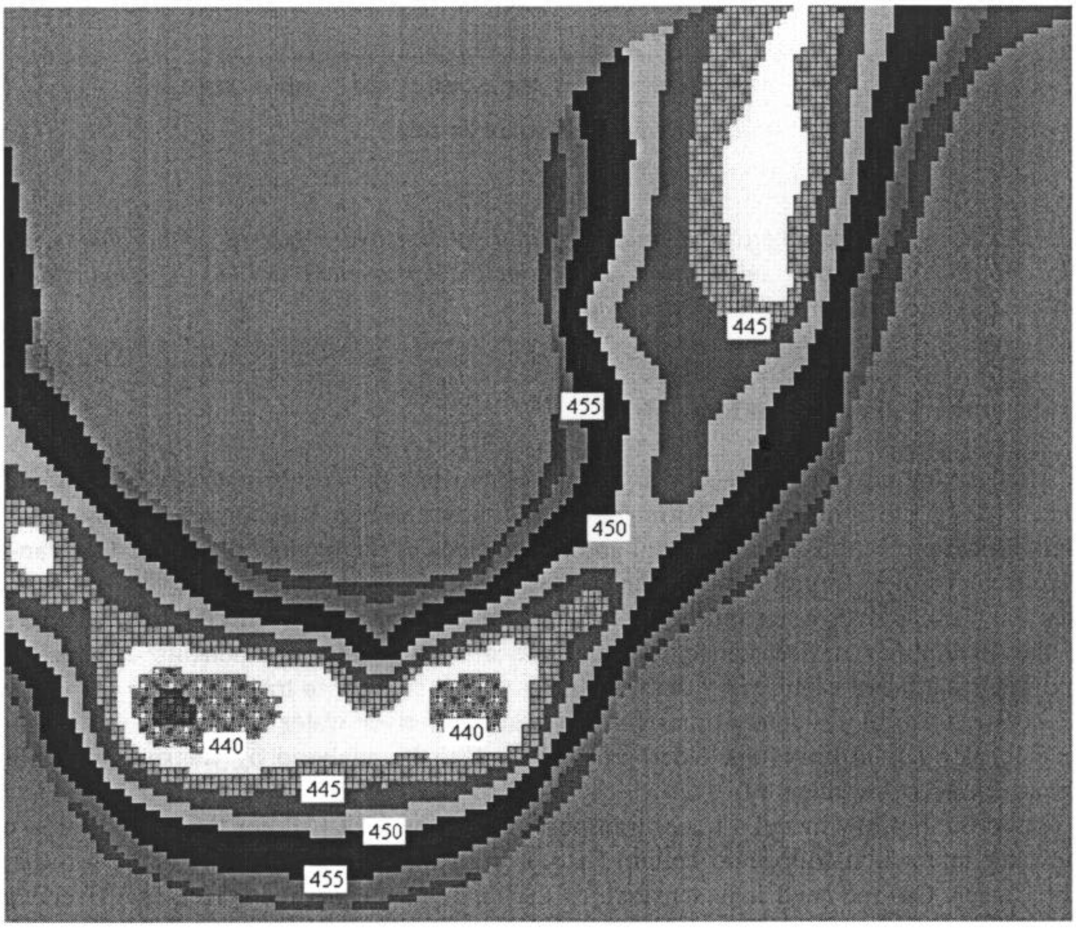


Fig. 2: Topography of the lower boundary of the aquifer interpolated from the top levels of the Molasse layer observed in the boreholes. The numbers represent the elevation of the contour lines in m amsl. The maximum thickness of the aquifer amounts to 20 - 25 m.

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 aquifer and the river water levels along the river course as well as the hydraulic conductance of the river bed. The latter depends strongly from the state of clogging of the river bed and can vary in space and time.

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 (Fig. 3). No unique solution was found. However, good fits were obtained for values centered around $3 \cdot 10^{-4}$ m^2/s for the conductance of the river bed, $2 \cdot 10^{-3}$ m/s for the higher and $2 \cdot 10^{-5}$ m/s for the lower horizontal hydraulic conductivities.

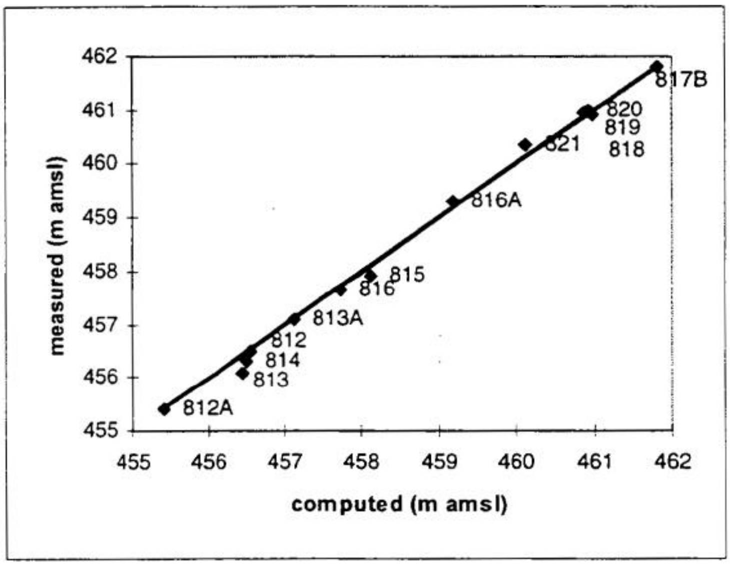


Fig. 3: Deviation between measured and computed piezometric heads of 13 boreholes within the model area after steady-state calibration. The estimated parameters include the conductance of the river bed as well as two hydraulic conductivities.

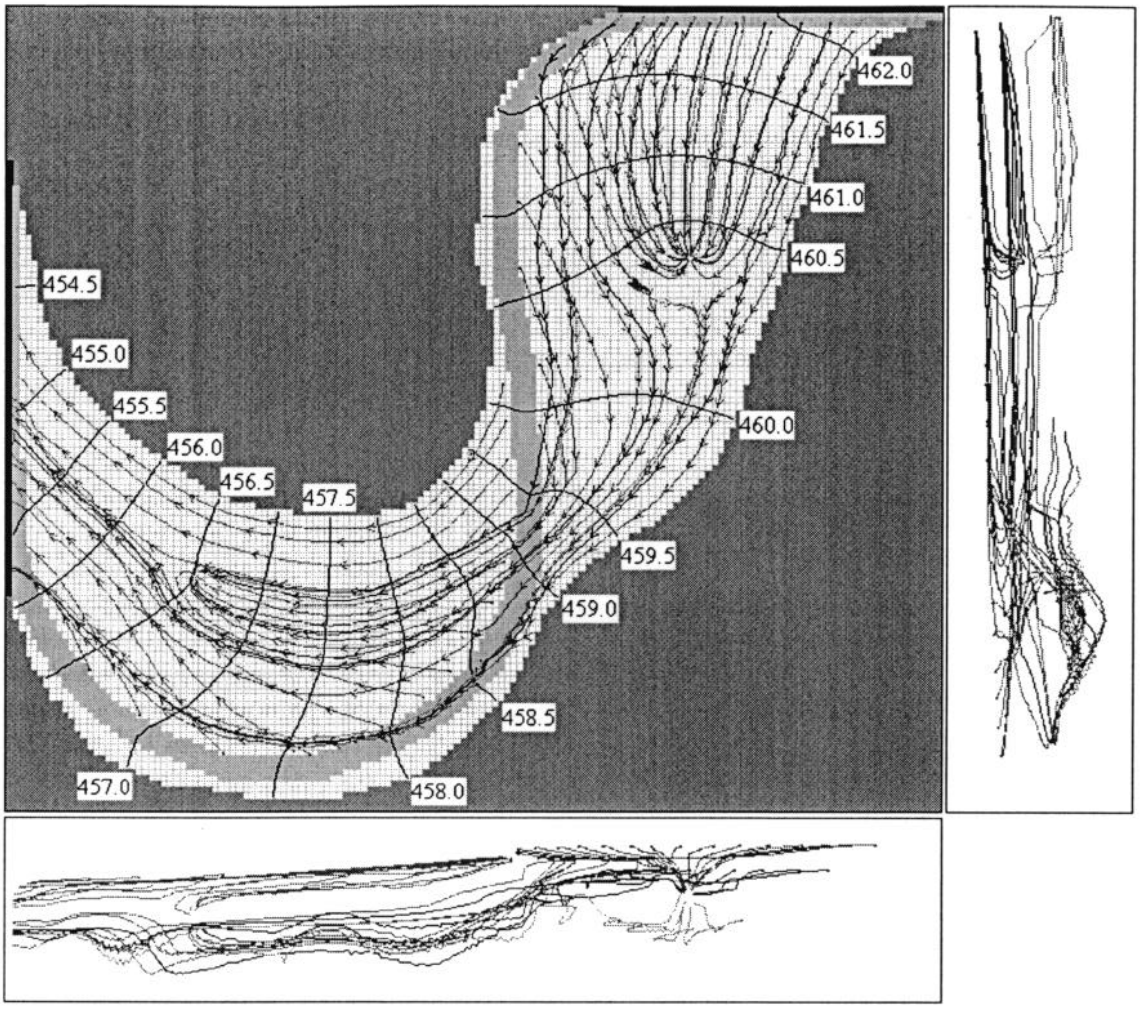


Fig. 4: Streamlines for steady-state conditions shown as horizontal projections on the top and vertical projections on the frontal and lateral sides of the modelled volume. The numbered black lines represent the isolines of the water table elevation in the top layer of the aquifer (m amsl). Streamlines are entering the aquifer from the river cells of the upper and the lower river loop and from the 'fixed head' cells of the upstream model boundary. Neighbouring arrows on the streamlines mark a time interval of ten days.

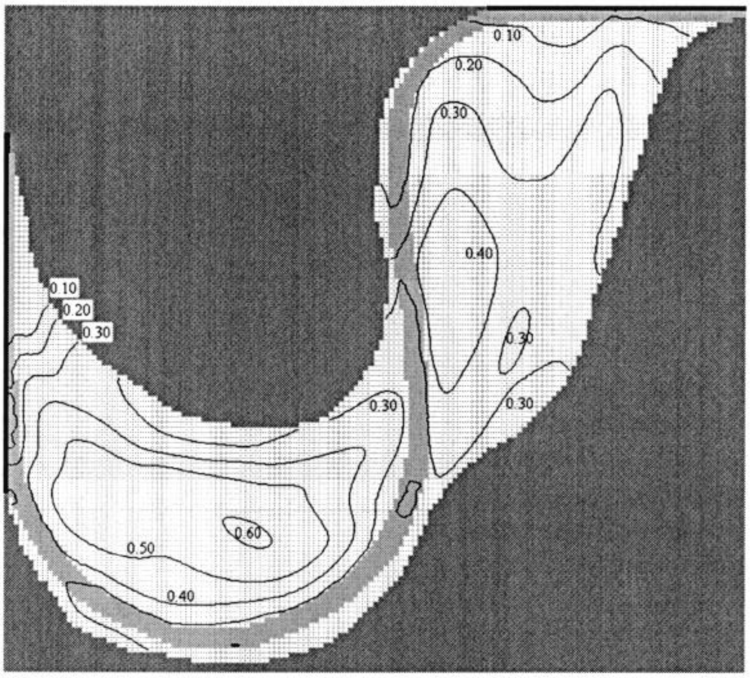


Fig. 5: Distribution of $^3He_{tri}$-concentration in the top layer of the aquifer originating from tritium decay within the model area. The black lines represent the isolines of concentration and the numbers the corresponding numerical values of the concentration in 10^{-15} $cm^3STP \cdot g^{-1}$.

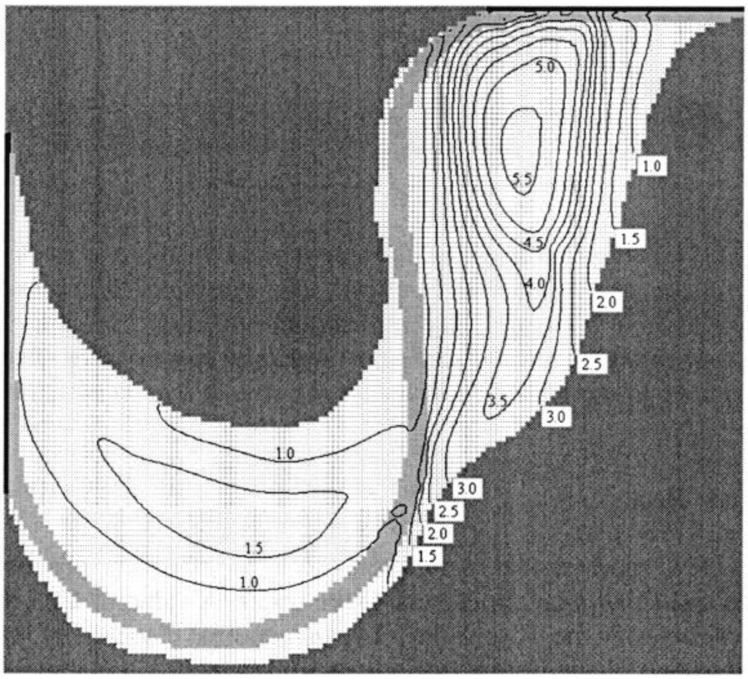


Fig. 6: Distribution of the total $^3He_{tri}$-concentration in the top layer of the aquifer (accumulation by tritium decay as well as amount imported via the upstream model boundary). The black lines represent the isolines of concentration and the numbers the corresponding numerical values of the concentration in 10^{-15} $cm^3STP \cdot g^{-1}$.

4. Results of the 3-dimensional Flow Model

After having provided the necessary model parameters the steady-state flow conditions can be calculated [3, 4]. The 3-dimensional streamlines are shown in Fig. 4 as horizontal projections on the top and vertical projections on the frontal and lateral sides of the modelled volume. One can see that both wells pump deeper groundwater entering the modelled domain through the upstream model boundary as well as river water infiltrated in the vicinity of the wells. With the help of time markers along the streamlines the residence times of the different water components can be estimated. 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 of a conservative tracer (see chapt. 6).

Based on the flow model a tracer transport model was built [5]. For the investigation of river-groundwater interaction tritiogenic helium ($^3He_{tri}$) originating from the decay of ^3H proved to be a valuable tracer. 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. Therefore successful modelling of this tracer does not only confirm the mixing ratios between river water and groundwater but also the velocities of the flow model.

5. Results of the Transport Modeling of $^3He_{tri}$

Transport modelling requires a few more model parameters 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 reasonable for the Toss 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 [6]. For transport over distances between 100 m 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 appropriate for the present transport model. As a noble gas, ^3He does not undergo degradation nor retardation caused by adsorption. Instead, the ingrowth of ^3He by decay of tritium must be taken into account, especially if the residence times are not negligible compared to the half-live of ^3H (about 12.3 years).

The result of the transport model is a spatial distribution of tracer concentrations. Fig. 5 shows the distribution of $^3He_{tri}$ originating from tritium decay within the model area, while Fig. 6 shows the total $^3He_{tri}$ including the amount imported via the upstream model boundary. A comparison of the two figures shows that ^3H-decay within the model area adds only a small amount to the total ^3He-concentration in the upper river loop; in the lower loop, however, its contribution amounts to up to 40 %.

Comparing the calculated $^3He_{tri}$-concentrations of the two wells with the measured concentrations (Table I), one obtains a good correspondence for „Sennschür“. The computed value for „Obere Au“ is, however, too low by about 40 %. Possible reasons could be:

- The well obtains more $^3He_{tri}$-free river water in the model as a result of a too high estimated value for the hydraulic conductance of the river bed,
- the $^3He_{tri}$-rich deeper groundwater is diluted too strongly 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 too small), leading to too low an accumulation of $^3He_{tri}$ by ^3H-decay.

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

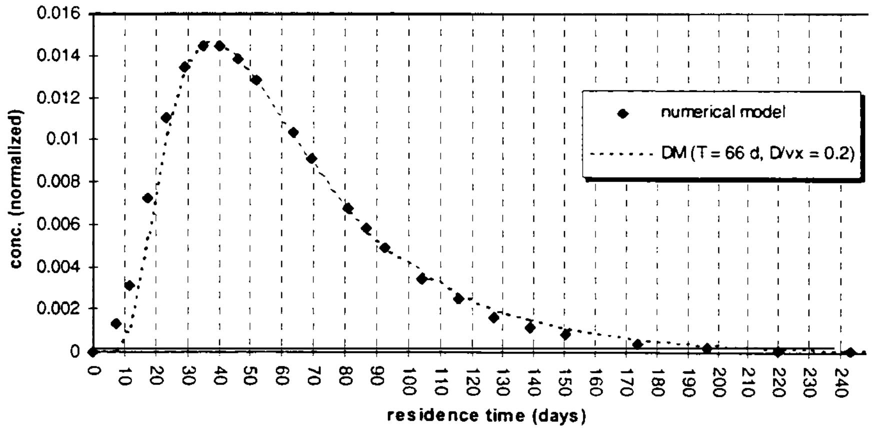
TABLE I: MEASURED AND COMPUTED CONCENTRATIONS OF TRITIOGENIC ^3HE ($^3HE_{TRI}$) FOR THE TWO WELLS „SENNSCHÜR“ AND „OBERE AU“ FOR TWO DIFFERENT VALUES OF THE RIVER BED CONDUCTANCE.

Pumping Station	$^3He_{tri}$ computed conductance = $3\cdot10^{-4}$ m²/s ($cm^3STP\cdot g^{-1}$)	$^3He_{tri}$ computed conductance = $1\cdot10^{-4}$ m²/s ($cm^3STP\cdot g^{-1}$)	$^3He_{tri}$ measured ($cm^3STP\cdot g^{-1}$)
„Sennschür“	$5.08\cdot10^{-15}$	5.46.10-r’	$(4.9 \pm 1.0)\cdot10^{-15}$
„Obere Au“	$1.60.\ 10^{-15}$	$2.27\cdot10^{-15}$	$(2.8 \pm 0.9)\cdot10^{-15}$

6. 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 δ-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 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 to determine the mixing ratios in the wells (see below).

Comparing the normalized break-through curves calculated by transport modelling with a spectrum of residence times of a dispersion model, as it is often used for the interpretation of environmental radioisotopes (see e.g. [7]), one gets good correspondance for the river water component in the well „Sennschür" (Fig. 7). 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, 7: Normalized break-through curve of a conservative tracer computed for well „Sennschür " as response to a δ-pulse to river cells (diamonds). The computed curve can be compared with the spectrum of residence times (dotted lines) of a two-parameter dispersion model (mean residence time T and dispersion parameter D/vx).

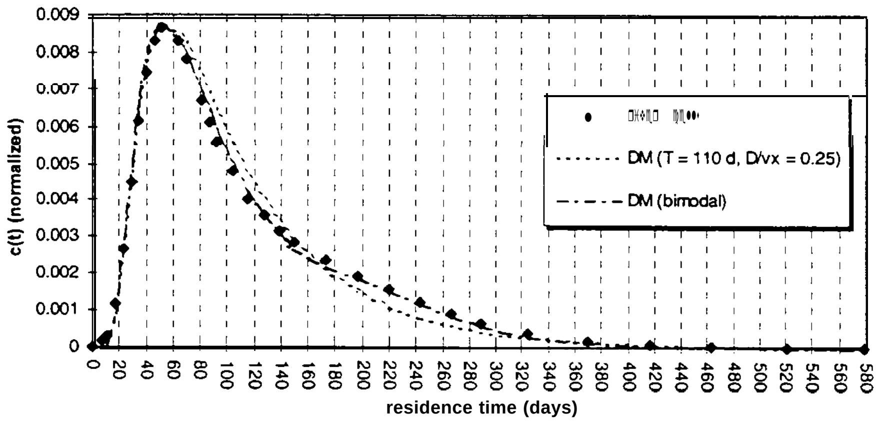


Fig. 8: Normalized break-through curve of a conservative tracer computed for well „ Obere Au" as response to a &pulse input to river cells (diamonds). Because of the mixture of river water components with different mean residence times the computed break through curves cannot be reproduced by a simple box model. The resulting bimodal distribution of residence times could only be reproduced by two dispersion models in parallel respecting the exact mixing ratios.

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 (Fig. 8). This shows the advantage of the spatially 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 infiltrated river water calculated by means of the non-normalized break through curves (Fig. 9) 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 $^3He_{tri}$ 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 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 $^3He_{tri}$ in the wells on the other hand allow a sensitive calibration of this parameter. With a conductance slightly decreased by a factor of 3, the measured concentration of $^3He_{tri}$ 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 I).

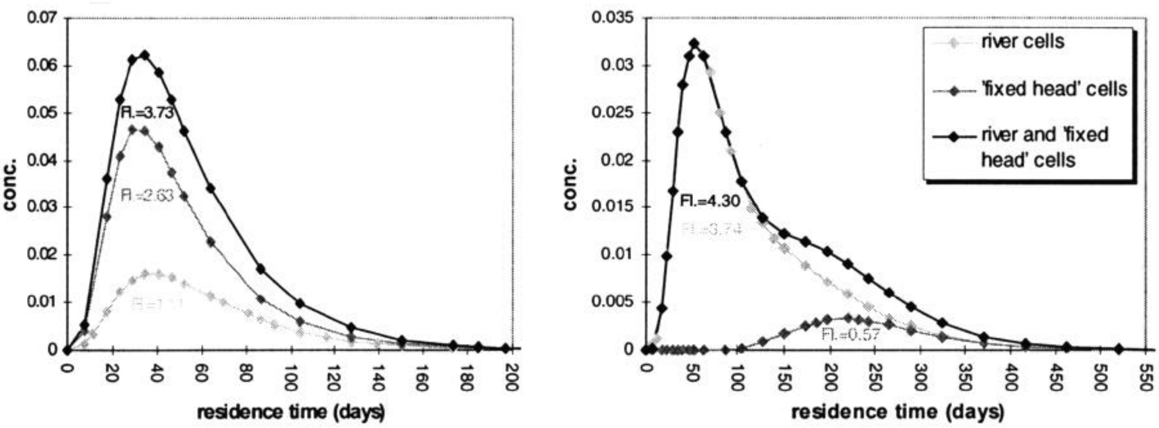


Fig. 9: Non-normalized break-through curves of a conservative tracer computed for wells „Sennschür“ (left) and „Obere Au“(right) as response to a δ-pulse input to different inflows to the aquifer. The area below the curves (given by the numbers) is equivalent to the amount of tracer being recovered by the wells from the different inflow sources and is used to obtain the mixing ratios in the wells.

7. Conclusions

The flow model presented in this study is based on a conceptual sedimentological model that allows to reduce the number of free model parameters. 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. The conceptual sedimentological model only represents the major structure and cannot reproduce local properties of the aquifer.

Transport modelling of tritiogenic ^3He clearly showed that the most important parameter for the river-groundwater system is the conductance of the river bed. 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.

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