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On the use of spring baseflow recession for a more accurate parameterization of aquifer transit time distribution functions

J. Farlin[1] **and P. Maloszewski**[2]

[1]Centre de Ressources des Technologies de l'Environnement,
Centre de Recherche Public Henri Tudor, Luxembourg
[2]Institute for Groundwater Ecology, Helmholtz Centre Munich, Germany

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Correspondence to: J. Farlin (julien.farlin@tudor.lu)

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Abstract

Baseflow recession analysis and groundwater dating have up to now developed as two distinct branches of hydrogeology and were used to solve entirely different problems. We show that by combining two classical models, namely Boussinesq's Equation describing spring baseflow recession and the exponential piston-flow model used in groundwater dating studies, the parameters describing the transit time distribution of an aquifer can be in some cases estimated to a far more accurate degree than with the latter alone. Under the assumption that the aquifer basis is sub-horizontal, the mean residence time of water in the saturated zone can be estimated from spring baseflow recession. This provides an independent estimate of groundwater residence time that can refine those obtained from tritium measurements. This approach is demonstrated in a case study predicting atrazine concentration trend in a series of springs draining the fractured-rock aquifer known as the Luxembourg Sandstone. A transport model calibrated on tritium measurements alone predicted different times to trend reversal following the nationwide ban on atrazine in 2005 with different rates of decrease. For some of the springs, the best agreement between observed and predicted time of trend reversal was reached for the model calibrated using both tritium measurements and the recession of spring discharge during the dry season. The agreement between predicted and observed values was however poorer for the springs displaying the most gentle recessions, possibly indicating the stronger influence of continuous groundwater recharge during the dry period.

1 Introduction

Spring baseflow recession analysis began more than a century ago when Boussinesq and Maillet, who proposed using quadratic or exponential laws to approximate the shape of spring recession (Boussinesq, 1904; Maillet, 1905). Following this seminal work, a number of more complex models have been developed combining two or more

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reservoirs and considering non-linear responses (Horton, 1933; Brutsaert and Nieber, 1977; Brutsaert, 1994; Coutagne, 1948; Mangin, 1970; Padilla et al., 1994). Dewandel et al. (2003) give an excellent review of the subject, and separate all recession studies into two approaches: the first considering drainage in both saturated and unsaturated zones, and the second concentrating on the recession of the saturated zone only. For the latter, only Boussinesq's quadratic solution is both analytically exact and interpretable hydrodynamically. As was shown from the statistical analysis of 100 karstic recessions (Drogue, 1972) and using numerical techniques (Dewandel et al., 2003), a quadratic law describes much more truthfully spring recession than an exponential law, although the latter has proven more popular in groundwater hydrology. Furthermore, the quadratic law, although derived from a number of simplifying assumptions, proved robust for more realistic aquifers. Acknowledging this, we adopted Boussinesq quadratic law to describe spring flow recession.

One of the reasons to study baseflow recession is that since its shape is controlled by the hydrodynamic properties and geometry of the aquifer, it is possible to estimate from the discharge recession an averaged (so-called effective) hydraulic conductivity and storage coefficient (Boussinesq, 1904; Brutsaert and Nieber, 1977; Brutsaert, 1994; Szilagyi et al., 1998; Mendoza et al., 2003). Since the equation relates the volume of water in storage and spring discharge, the mean hydraulic residence time in the saturated zone is another parameter that can be derived from fitting the Boussinesq quadratic solution to an observed spring recession (but one which did not receive much attention until now).

Mean groundwater residences times are usually estimated using lumped-parameter models (Maloszewski and Zuber, 1982) calibrated on the measurement of environmental tracers such as tritium or CFCs. Since tritium infiltrates conservatively with rainwater, the estimated residence time is the sum of residence times in the unsaturated and saturated zones. Due to the shape of the tritium input function, the solution of the inverse estimation can be non-unique, especially for residence time distributions with more than one parameter or when the tritium record in the outlet is short. If the model is

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used to predict solute transport time, this non-uniqueness is propagated to the results of the solute transport model.

In this paper, we show that the discharge recession can be used to reduce parameter uncertainties in a model predicting atrazine concentration in spring water over time.The parameters of the model are estimated from tritium measurements and baseflow recession, and predictions then compared with the observed atrazine time series in a second verification/falsification step.

2 Material and method

Both methods used in this study fall under are convolutions predicting the answer (output) of an environmental system to a particular input by means of a transfer function. Besides being used to estimate groundwater residence times, convolutions have been applied in the field of hydrogeology to estimate groundwater recharge as well as the transfer function of the unsaturated zone (Besbes and de Marsily, 1986) and study water table fluctuations (Olsthoorn, 2008). The physical meaning of the transfer function adopted varies between applications and may even be chosen purely empirically. Both the EPM and Boussineq's quadratic function however are exact analytical solutions, the former describing the residence time distribution of flowlines in a homogeneous aquifer and the latter resulting from the integration of the diffusion Equation under a set of simplifying assumptions.

2.1 Atrazine residence time and prediction of spring water atrazine concentration

The model predicting atrazine concentration in spring water over time is based on the transit time distribution of the aquifer, representing the sum of flow through all flowlines connected to the outlet, each characterized by its particular transit time. The transit time distribution function used here is the exponential piston-flow model (EPM) proposed by

Maloszewski and Zuber (1982), a combination of two simpler models, piston-flow and exponential. The piston-flow component simulates the thick unsaturated zone where all flow lines are approximately vertical and of equal length and transit time (Farlin et al., 2012), and the exponential component the transit time distribution in the saturated zone. The EPM has two fitting parameters (which can be expressed as the mean residence time in the unsaturated and saturated zones respectively).

Atrazine concentration in spring water $C_{\mathrm{out}}$is predicted from the input leaching concentration C_{in} by (Farlin et al., 2012)

$$C_{\mathrm{out}}(t) = \frac{x_{\mathrm{cropland}}}{x}\int_{-\infty}^{t} C_{\mathrm{in}}(\tau)\, g'(t-\tau)\exp[-\lambda(t-\tau)]\mathrm{d}\tau \tag{1}$$

The model assumes atrazine behaves conservatively in the aquifer (i.e. sorption and degradation processes are negligible). The transit time distribution $g'(\tau)$ is different from the transit time distribution of tritium $g(\tau)$ due to the fact that atrazine is only applied on agricultural surfaces, whereas tritium infiltrates homogeneously over the entire recharge area. Both functions are however functionally related, and the parameters of $g'(\tau)$ can be estimated from those of $g(\tau)$, provided the land-use distribution is known (Farlin et al., 2012). $g(\tau)$ is defined by Maloszewski and Zuber (1982) as follows

$$\begin{aligned} g(\tau) &= \frac{\eta}{t_{\mathrm{epm}}}\exp\left(-\frac{\eta\tau}{t_{\mathrm{epm}}}+\eta-1\right) \quad \text{for} \quad \tau \geq \frac{\eta-1}{\eta}t_{\mathrm{epm}} \\ g(\tau) &= 0 \quad \text{for} \quad 0 < \tau < \frac{\eta-1}{\eta}t_{\mathrm{epm}} \end{aligned} \tag{2}$$

with $\eta =$ ratio of total volume of water in the stored groundwater system (V) to the volume of water stored in the reservoir with exponentially distributed of transit times (V_{EM}) [–]

$$\eta = \frac{V}{V_{\mathrm{em}}} = \frac{t_{\mathrm{epm}}}{t_{\mathrm{epm}} - t_{\mathrm{pf}}} = \frac{t_{\mathrm{epm}}}{t_{\mathrm{em}}} \tag{3}$$

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t_{epm} = total mean residence time of the tracer in the system (in a double porous medium), t_{pf} = mean residence time of the tracer in the unsaturated zone and t_{em} = mean residence time of the tracer in the saturated zone.

Both parameters of the EPM are a priori unknown and must be estimated from environmental tracer measurements (tritium in the present study, see Farlin et al., 2012, for details). The goodness of fit is calculated from the misfit between predicted and observed tritium concentrations

$$\varepsilon = \sqrt{\sum_{i=1}^{N} \left[C_{\mathrm{obs}}(t_i) - C_{\mathrm{mod}}(t_i)\right]^2 / N} \qquad (4)$$

The best fit is obtained by minimizing of ε (with a visual verification). Theoretically, both t_{epm} and η can be estimated from tritium data. However, in practical applications, η is not always a sensitive parameter and in some cases cannot be constrained precisely using tritium measurements only, different values yielding equally good fits both numerically and visually. In other words, the total mean residence time can be estimated, but not separated into its components t_{em} and t_{pf} (respectively residence time in the saturated and unsaturated zone). For that reason, we try to estimate η from the recession hydrograph.

2.2 Recession curve analysis

Boussinesq (1904) derived an analytical solution of the flow equation for an aquifer with a horizontal basis. Recession follows then a quadratic law

$$Q(t) = \frac{Q(t_0)}{(1+kt)^2} \qquad (5)$$

with Q = discharge [$\mathrm{L}^3\,\mathrm{T}^{-1}$], t_0 = begin of the recession [T] and k = recession coefficient [T^{-1}].

The volume of water in storage at any time t is (Drogue, 1972)

$$V(t) = \frac{Q(t)}{k} \tag{6}$$

According to Maloszewski and Zuber (1982) the mean residence time in the saturated zone (the turnover time) is

$$t_{\mathrm{em}} = \frac{V_{\mathrm{mean}}}{Q_{\mathrm{mean}}} \tag{7}$$

Comparing Eqs. (6) and (7), we see that

$$t_{\mathrm{em}} = \frac{1}{k} \tag{8}$$

Knowing t_{em} from the recession and t_{epm} from tritium observations, Eq. (3) can be used to estimate η.

Mean residence times in the saturated zone calculated from a tracer and from the recession will be approximately equal if and only if zones of stagnant water are negligible. Stagnant zones can be present in double porous systems with active diffusion into the matrix. A second possible situation is when the basis of the aquifer is convex, causing the trajectory of some flowlines to plunge below the aquifer outlet and creating a groundwater reservoir (referred to by Zuber, 1986, as the minimum volume) that does not influence the discharge rate because it is situated deeper than the outlet. In that case, the recession only informs on the residence time of the dynamic volume (the volume of water stored above the datum of the outlet), whereas tracer residence times will be calculated for the sum of dynamic and minimum volumes. Hence, two assumptions have to be made when combining tracer information with hydrograph recession, both related to the different storage volumes existing in the aquifer. The first is that even in double porous aquifers, the matrix porosity is nearly inactive for both water and tracer exchange. The second is that the basis of the aquifer is sloping continuously

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towards the outlet or is at most horizontal. In cases where the matrix porosity cannot be neglected, the comparison between mean residence times in the saturated zone calculated from tritium and from the recession can allow to estimate the ratio matrix porosity to total porosity.

The recession analysis also suffers from one major limitation. When groundwater recharge is not negligible during the dry period, the observed discharge recession does not give the "true" recession coefficient, as the aquifer is influenced by additional water inflow. This leads to an over estimation of the mean hydraulic residence time and an underestimation of η. Corrections taking the effective net infiltration into account during the dry period may partially solve this issue, but have not been looked into yet.

All these elements must be kept in mind during data analysis.

2.3 Study area

A series of springs draining the Steinsel plateau, a sandstone cuesta situated ten kilometers north of Luxembourg City, were sampled regularly over three years (2008 to 2011). The plateau is part of a fractured sandstone aquifer named the Luxembourg Sandstone which provides about half of the country's drinking water. The formation is densely fractured, and has a thickness of up to a 100 m with a large unsaturated zone. Few measurements exist for both matrix and fracture porosities. The former varies with the degree of dissolution of the calcareous cement (from 5 % to 35 % according to Colbach, 2005). Fracture porosity is estimated by the same author to be approximately 1 %, but Farlin et al. (2012) calculated from the mean groundwater residence time, the mean annual recharge and the thickness of the saturated and unsaturated zones fracture porosity values between 5 and 6 % for the Steinsel plateau nearly accounting for the entire active porosity.

The springs were sampled either weekly or monthly from 2008 to March 2010, and thrice in 2011. Sampling included water chemistry and pesticide concentrations. pH, electric conductivity, water temperature as well as spring discharge were measured in the field. Tritium was measured twice each year in July and September. The water quality of many springs draining the Luxembourg Sandstone, including those sampled, is impacted by intensive farming practices taking place in recharge areas. The mean groundwater residence times were estimated from tritium measurements using the EPM, and were found to be approximately equal to 15 yr. Equation (1) was developed to predict the evolution of atrazine concentration in spring water following its countrywide ban in 2005. Atrazine concentrations were stable until 2011, where the beginning of a decreasing trend was observed. This prompted to return to the original predictions made based solely on the data from 2008–2010 and to assess with hindsight the model's predictive power. The original model presented in Farlin et al. (2012) was sufficient to explain the inertia of the aquifer system and estimate approximately the time to trend reversal. It suffered however from two major flaws: different stages of atrazine application practices were ignored (leaching from the soil being represented by a step function simulating a constant leaching over decades followed by the 2005 ban) and the tritium data were not sufficient to differentiate between two models predicting different mean residence times in the saturated and unsaturated zones (for the same total residence time within the formation).

3 Results

3.1 Spring recession

Most springs displayed a clear recession lasting from February till as late as June. Table 1 summarizes the t_{em} estimated from the recession periods in 2008 and 2009. The parameter estimation is performed by least-square fitting, with both $Q(t_0)$ and k allowed to vary. For some springs, both years yield comparable mean residence times in the saturated zone, but for others (K17, K21 and K21a) estimates differ by a factor two between 2008 and 2009, with the shorter residence time closer to those in the other springs. Note that the recession in 2008 nearly systematically yields longer mean residence times than the recession in 2009 (with the exception of K17 and to a much lesser extent K9). Discharge time series and quadratic fit are shown exemplarily for three springs on Fig. 1, each illustrating one type of recession (nearly identical in both years, some additional influence during the dry period in one of the two years, and a large influence during the dry period).

3.2 Atrazine concentration

The history of atrazine soil application was unknown except for two dates. The first was the introduction of combination products in the early nineties which made overdosing atrazine impractical, as this simultaneously increased the dose of other products present in the formulation, damaging the treated crops. The second date was the nationwide ban on atrazine which was enforced in 2005. Hence, we can at least reconstruct a schematic history of atrazine leaching to the groundwater in three stages. A first stage of higher leaching until the mid-nineties, followed by decreased leaching up to around 2005 (taking into account a certain lag until farmers had exhausted their atrazine stock and the atrazine reservoir in the soil had been sufficiently depleted), and a third stage consisting of atrazine-free recharge water. Thus, the predictive model consisting of Eq. (1) was used with a time series C_{in} consisting of a single step function with a break placed in the mid-nineties. In first approximation, we assumed the leaching during the combi-product period much smaller and negligible compared to the leaching of the pure atrazine phase. The parameters of $g(\tau)$ were estimated both from tritium measurements alone, yielding two different models (models “tritium 1” and “tritium 2”), and tritium combined with spring baseflow recession (model “recession”). Depending on the data available, one or two recession models were used (corresponding to a parameter k estimated from the recession in 2008 and 2009 respectively). Finally, the break in C_{in} was shifted until the best agreement was reached between model predictions and observations. This additional fitting step was necessary for two reasons: the shift by farmers from pure atrazine to combination product probably did not take place instantly, and the soil acts as an additional reservoir that reacts to changing application practices with a lag of a few years (Farlin et al., 2012). The final predictions are shown

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on Fig. 2. Model 2 displays a quicker reaction to change than model 1, reflecting the larger piston-flow component ($\eta = 5.9$ and 4.4 respectively for K17).

A comparison of the different models predicting atrazine concentration over time is shown for the same three springs as above on Figs. 3, 4 and 5. For the models fitted using the recession, the shortest t_{em} value of each spring (Table 1) was used for parameter estimation. The uncertainty interval shown only reflects the uncertainty of the agricultural fields to total recharge area ratio which is one parameter of $g(\tau)$ (see Farlin et al., 2012, for details). The selected springs illustrate three different cases. In the first case (Fig. 3), η can be estimated uniquely from tritium data and model predictions made using either tritium only or tritium in combination with the recession curve are nearly identical. Estimates made from the tritium measurements give mean groundwater residence times of approximately 15 yr, and indeed, the decrease in atrazine concentration observed after 2010 can be traced back to the end of the nineteen nineties, i.e. to the shift from pure atrazine to combination products. In the second case (Fig. 4), only one of the two tritium models predicts correctly the atrazine decrease. The η value of this model is also close to the estimate made using the recession. For the third example (spring K2), atrazine concentration in 2011 was still within the range observed in the period 2008–2010. Consequently, because the information content is poor, and although η estimates from the recession and one tritium model are close to one another (2.4 versus 2.9), none of the models performs clearly better in predicting the atrazine evolution over time.

4 Discussion

The purpose of the study presented here was to combine information concerning hydraulic residence times and tracer residence times into a consistent model. As could be shown, this approach is useful to reduce the number of possible models obtained from tritium measurements by rejecting those that do not agree with independent observations of spring baseflow recession.

In the case study presented the influenced recession constitutes the main limitation to the method. As shown in Table 1, residence times calculated from the recession are with two exceptions longer in 2008 than in 2009. This correlates qualitatively with rainfall, 2008 having been a wetter year than 2009. Springs larger than those draining the Luxembourg Sandstone or situated in more arid climates may be less sensitive to a small recharge rate during the summer months, as for instance in the ophiolite hard-rock aquifer presented by Dewandel et al. (2003). A pragmatic solution is first to inspect first the shape of the recession and look for irregularities not explainable by measurement error, and secondly to adopt the steeper recession observed for a spring as the closest approximation to a perfect uninfluenced recession (which may never be observed in shallow aquifers in temperate climates). Deviations limited in time due to fast flow are less problematic than continuous recharge, since fast flow water does not reach the groundwater table but travels laterally down slope without modifying the hydraulic gradient in the saturated zone, and thus leads to a temporary increase in the discharge but does not shift the entire recession limb upwards.

Applying model-based corrections may constitute a workable alternative, with the effective precipitation calculated from a bucket model serving as input for a simple reservoir model parameterized using Eqs. (3) and (4). The fit could thus be performed on the entire time series, and not just on the recessions, a particular advantage for longer records. By that means it would be possible to include recharge dynamics into the model, which would make it more comprehensive, but also more complex.

The agreement between η estimates from recession and tritium is an indication that the dynamic volume could be nearly equal to the total volume of water stored in the saturated zone, in other words that fracture porosity would nearly completely account for the total porosity of the Luxembourg Sandstone. This agrees with previous estimates made from tritium measurements alone by Farlin et al. (2012). In groundwater systems where diffusion into the rock matrix cannot be neglected, comparing η thus provides a way to calculate tritium retardation and consequently calculate the ratio of dynamic to total porosity.

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5 Conclusions

We have shown here that a quantitative analysis of aquifer baseflow recession can constrain the parameter range of a transit time distribution function, contributing to reduce the prediction uncertainties of a model describing atrazine evolution in spring water over time. Simple to measure and thus often readily available, spring discharge can provide extremely useful information on the integrated hydraulic response of the aquifer to recharge dynamics. Groundwater systems dominated by slow flow are particularly suited, since distortions of the baseflow recession caused by fast flow is minimum.

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Table 1. t_{em} estimated from Eq. (8) for the observed recessions in 2008 and 2009.

	t_{em} [yr]		median
Spring	2008	2009	discharge [L min^{-1}]
K1	4.57	4.57	158
K2	5.48	3.91	156
K3	6.85	–	59
K4	3.04	2.11	23
K5	6.85	5.48	41
K7	3.04	–	298
K9	2.11	2.49	10
K16	2.74	–	7
K17	3.91	9.13	76
K19	4.57	–	85
K21	6.85	3.04	187
K21a	13.7	2.74	42

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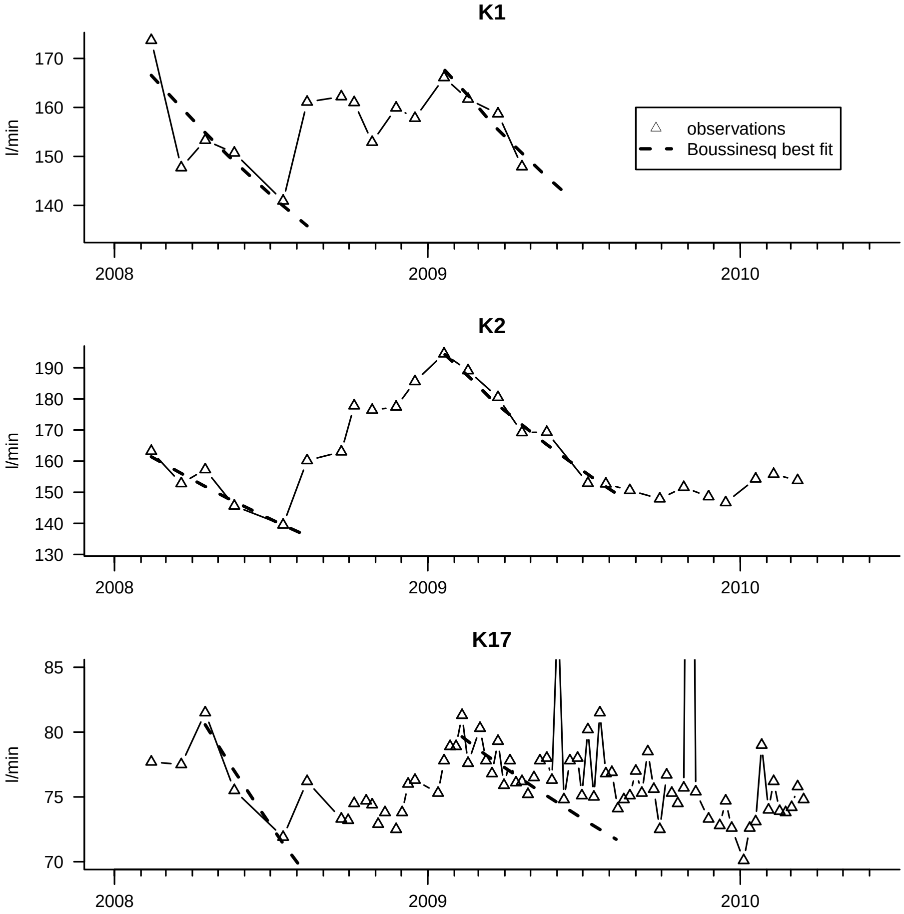

Fig. 1. Discharge measurements and best fit of the quadratic recession.

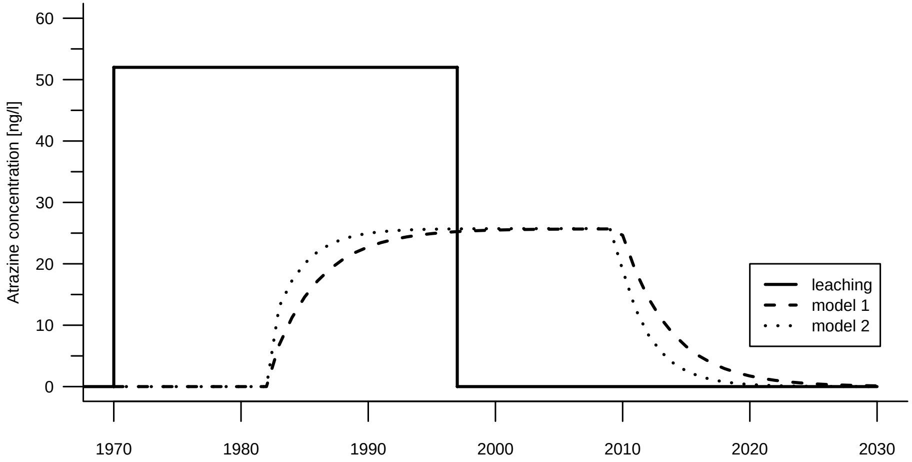

Fig. 2. Atrazine leaching input and output time series (K17). The duration of the leaching period was adjusted to agree with the atrazine decrease observed in the springs (Figs. 3, 4 and 5).

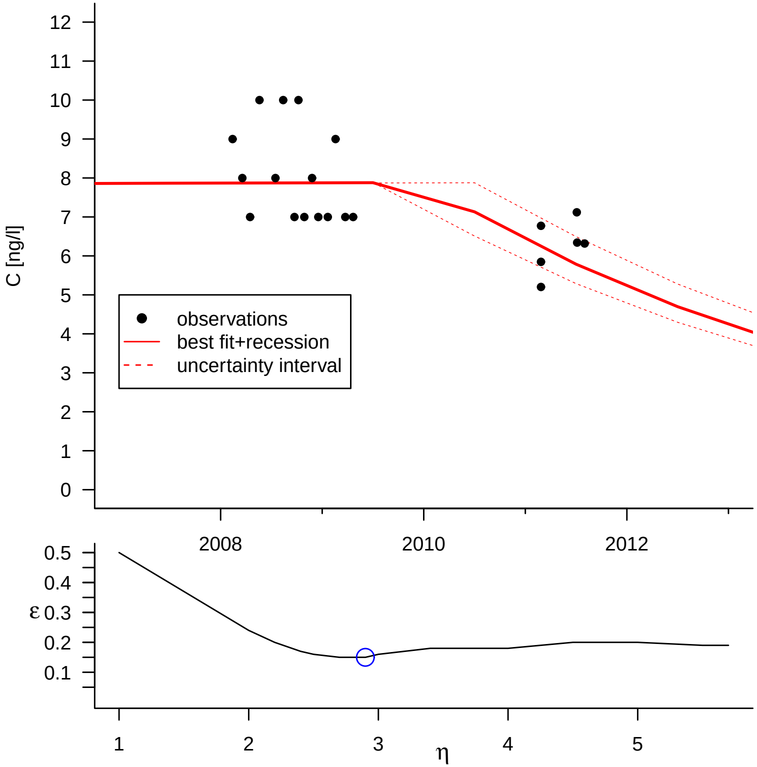

Fig. 3. Model prediction of atrazine concentration (top graph) and model error as function of η (bottom graph) for K1. The models with t_{em} estimated from tritium only or from the recession curve are nearly identical. η predicted from the discharge recession is shown by a blue circle, very close to the model error minimum (certainly the global minimum, since η values higher than 5.5 are physically unlikely).

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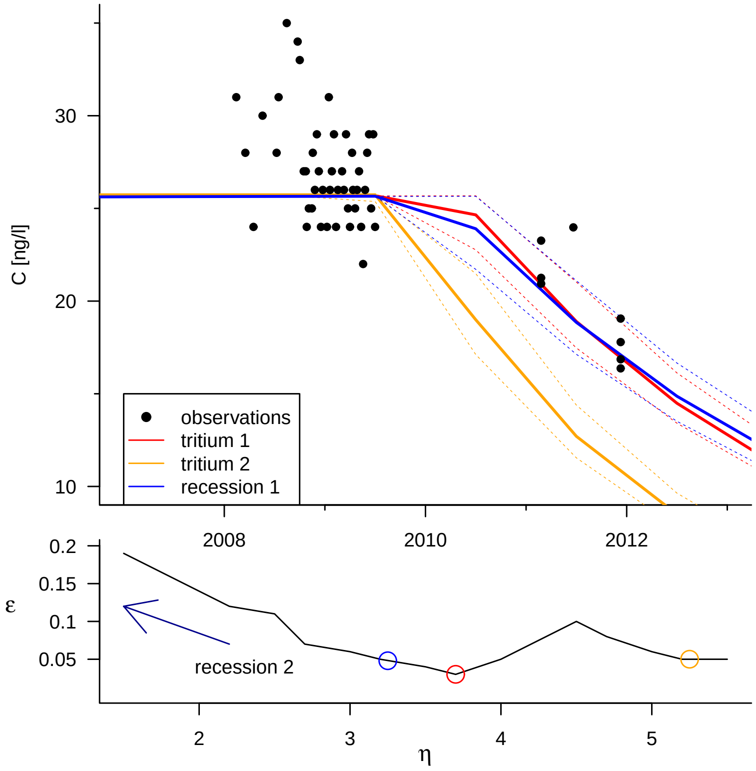

Fig. 4. Model prediction of atrazine concentration (top graph) and model error as function of η (bottom graph) for K17. η predicted by tritium model 1 is shown by a red circle, by tritium model 2 by an orange circle, and from the discharge recession by a blue circle. Based on the minimums of tritium model error, two models are nearly equally likely ($\eta = 3.7$ and $\eta = 5.2$). The first model however is closer to η predicted by the recession in 2008, and agrees better with observations. The recession observed in 2009 was obviously influenced, and lead to an estimate for η (1.5) much lower than estimates gained from tritium data.

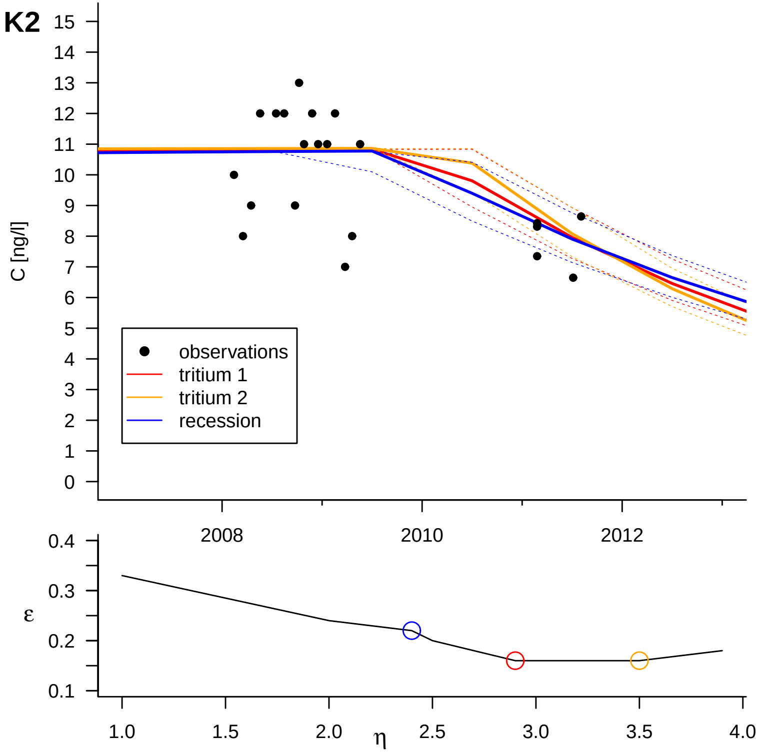

Fig. 5. Model prediction of atrazine concentration (top graph) and model error (bottom graph) for K2. η predicted by tritium model 1 is shown by a red circle, by tritium model 2 by an orange circle, and from the discharge recession by a blue circle. As for K17 (Fig. 3) two tritium models are equally likely ($\eta = 3.7$ and $\eta = 5.2$) with the first model closer to η predicted by the recession. Despite this, none of the models is clearly better at predicting the atrazine evolution over time.

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