Reply on RC2
Simon Hoeg

Author comment on "Benchmark tests for separating n time components of runoff with one stable isotope tracer" by Simon Hoeg, Hydrol. Earth Syst. Sci. Discuss., https://doi.org/10.5194/hess-2021-213-AC4, 2021

Dear Referee #2,

I appreciate your very positive and motivating feedback on my manuscript hess-2021-213.

> Author validated the iterative extension of standard two-component hydrograph separation method using a single isotopic signature (published in WRR in 2019) through a random rainfall generator and a rainfall-runoff model. I am happy to see that author has addressed a critical question raised during the WRR review why the new modeling approach did not overall improve the model’s uncertainty but instead increased uncertainties for some events. This current study confirmed the speculation at the time via "condition number" that it is the difference between new and old water that caused the increase in uncertainty. In addition, author demonstrated in the current study how the volume weighted separated event water response can serve as an estimator for a time-varying backward travel time distribution, which I consider is a novel contribution and will be of great interests to watershed hydrologists.

Thank you for summarizing the major outcomes.

> One defect in the design, however, is that ET (evaporation + transpiration) is entirely ignored in the rainfall-runoff model (Figure A2, though considered in equations 1 and 2), which is not realistic in the real-world scenario. It is unclear how consideration of ET will affect the modeling outcomes. Not to mention the impact of evaporation on isotopic fractionation (e.g., via bare soil evaporation and canopy interception), the influence of ET on streamflow quantity alone should affect the magnitude and timing of hydrograph and thus in my opinion possibly the isotopic signature of pre-event water, which is taken from streamflow right before an event. This defect will limit the application of this method to concept proofing and prevent it from broad application to real world-problem solving. But I am aware of the fact that adding ET impact in current study would make it way too complicated and extremely hard to follow. I think author should talk about any possible ET effect in a very general way in the current study and let readers be aware of its potential impact and explore whether or not this could be one of future studies. Additionally, I am curious if both isotopic tracers (2H and 18O) are used, whether or not isotopic fractionation due to evaporation and phase change can be incorporated into the
hydrograph separation model. If so, this would significantly boost its application and extend to snowmelt-dominated catchments.

Yes, ET and the impact of evaporation on isotopic fractionation is not explicitly considered in the current iterative separation equations. Instead, the effects of phase change on tracer concentrations would be subject to a Gaussian error analysis. Additionally, in the introduction I wrote that in the context of a chronological sequence of rainfall-runoff events, the event water concentration $c_e$ can be related to the tracer concentration in the precipitation $c_J$. This relation (e.g. $f: c_J \rightarrow c_e$) is always subject to certain assumptions, which are discussed in almost every hydrograph separation study. Based on function $f$, I would consider processes such as base soil evaporation and canopy interception when using the current model setup. In this numerical study, I have simply defined that $c_J = c_e$. However, mid and long term goal would be an extension of the current iterative mixing of the end members $Q_e, Q_{e-1}, ..., Q_{e-n}$ and $Q_p, Q_{p-1}, ..., Q_{p-n}$ towards an iterative splitting (see e.g. Kirchner and Allen (2020)) that would also explicitly include evapotranspiration processes.

> I do not think the current model is applicable to streamflow generated primarily from snowmelt.

If the quantity and isotope composition of snowmelt has been sufficiently monitored, then it can be also applied to the current model. In this case the above mentioned relation $f$ could be extended to $f(c_J, c_m) \rightarrow c_e$.

> I am also curious about the potential impact of prolonged droughts on the model results. What if there are two events that occur several months apart?

This is not a problem, as long as the age function remain stable (see e.g. line 155), that as long as piece-wise steady state conditions apply. If the age function has changed, which of course will happen in a prolonged drought, then it should be considered in the calculations. See also my comment at https://doi.org/10.5194/hess-2021-213-AC1

> Though I am not suggesting significant revisions to address the above issues in the current study, any potential impact and future extension should be discussed in the discussion section and the limitation should be cautioned in the conclusion section.

Yes, the discussion and conclusion section might additionally address the above mentioned topics.

> To promote this study and extend the use of the method, I suggest author to add more details to some of the mathematical equations. I have some questions on these equations (see below), which basically require clarification or more information.

P3/L77: The bracket not closed at the end?

Yes, it is not closed, since $[t_n, t_{(n+1)}[ \text{ would be the next semantic interval.}

> P3/Equation 3: The time factor is muted for all quantities in the equations. That is fine, but readers must be reminded that within an event isotopic signature in all components is assumed to be constant. This implicit assumption was discussed later in the discussion section, but I think this assumption should be explicitly stated here and then discussed later in the discussion section.

It is true that the intra-storm time variability is muted for the end member concentrations $c_e, c_{e-1}, ..., c_{e-n}$ and $c_p, c_{p-1}, ..., c_{p-n}$ in most of the simulations. However, on page 4, Criteria 2 and 3 say that the "event/pre-event component maintains a constant
isotopic signature in space and time, or any variations can be accounted for”. From line 458 on page 16, I discuss for the strong delayed fractions scenario that with an increasing proportion of rapidly mobilized pre-event water, such as Q_{(e-1)}, the pre-event water concentration c_p (assumed to be constant during the event) may decreasingly represent the bulk pre-event concentration of the considered control volume. Therefore, in https://doi.org/10.5194/hess-2021-213-AC1 and https://doi.org/10.5194/hess-2021-213-AC2 I demonstrate a reverse and time variable adaptation of the tracer concentrations c_e(e); c_{e-1}(e+1), ..., c_{e-3}(e+3) by piece wise equating Niemi’s left hand side. The mean deviation between the simulated event water response and separated event water response is then in a range of 1e-13% also for a large delayed fractions of event water alpha_max.

> P5/L122: Isn’t “sequential event water response” a better term than “separated event water response”?

Basically yes, but I wanted to emphasize that this variable is derived from a hydrograph separation. Therefore, I would like to keep the term.

> P5/Equation 12: Why does the integral start from negative infinite, not tin (in as subscript)?

Here, I simply adopted the notation of Niemi (1977). I have to say that it is the more exact reference, since Maloszewski and Zuber (1982) applied similar equations, but used the expression "exit age" instead of "injection time". Also Botter et al. (2011) used the notation of Niemi (1977). Later van der Velde (2012) or Harmann (2015) defined backward and forward approaches by using the actual time (t) instead of the injection time (t_in), in the context of an age ranked distribution of the water and associated components being based on cumulative probabilities. To answer your question: The integral itself may not start from t_in, as t_in is the integration variable, but in practice only the values c_j(t_in) * h(t - t_in) > 0 will play a role for the result.

> Why not dt but dtin instead? Need to explain. I have the same question for equation 15 in page 6.

The variable t refers to the actual time, however in the backward perspective we look back to the injection time t_in.

> P7/L188: As “condition number” appears for the first time in the text and is not a well-known term in hydrology, it needs either a reference or a further explanation or at least an indication it is being explained below.

I agree, here I could add the references of Stoer (1994) and Higham (1995). The latter is currently available free of charge from Elsevier.

> P8/Equation 23: It is unclear how the term after the plus sign is derived or defined.

The Landau notation is used to describe the asymptotic behavior, when approaching a finite or infinite limit value. The big O is used to indicate a maximum order of magnitude. Actually, equation 23 is not that often mentioned in the literature, therefore I will replace it by a more popular form that would be: \( \text{norm}(\Delta x) / \text{norm}(x) \leq \text{cond}(A) / (1 - \text{cond}(A) \text{norm}(\Delta A) / \text{norm}(A)) \text{norm}(\Delta A) / \text{norm}(A) \)

> P8/L208: What is gamma here? Explain.

Gamma is a scalar, a real number. The property \( \text{cond} (\gamma A) = \text{cond}(A) \) says that the size of the condition number for matrix A cannot determined by any scaling factor.
> **P8/Equation 24:** "f" should be better explained.

See also my response at https://hess.copernicus.org/preprints/hess-2021-213/#AC3: Equation 24 can be found at Deuflhard and Hohmann (2019) and holds for disturbances in matrix $A$, in which $f'(A)$ is the derivation of matrix $A$, also known as the Jacobian matrix. With equation 24, I wanted to emphasize that the norm of the first derivative of the matrix $A$ is also limited by its condition. This is interesting in terms of the Gaussian error propagation, in which the entries of $f'(A)$ are applied to the uncertainties of the known variables. This way I wanted to point out analytically that a basic Gaussian error analysis of the system $A*x = b$ would not produce different results than an analysis based on the condition number. Certainly, I could better describe this in the corresponding section. However, in section 4.2, I have written that an "ill-conditioned system will lead to larger gradients in a Jacobian matrix and to potentially higher errors in a Gaussian error propagation".

> **P11/L313:** ET was not considered, but why were precipitation and runoff not equal?

The simulation is stopped exactly after four years ($4 \times 365 \times 24$ hours). During the last time step the outflow $Q$ is still 0.08 mm, and the missing 2 mm belong to the storages $S_U$ and $S_L$.

> **P15/L411-421:** Need to mention that the current model setup does not work for snowmelt-dominated system.

I could mention that the current model setup has not been tested yet in snowmelt-dominated systems. Provided that the precipitation, snow layer and meltwater are adequately observed, I see no reason why it should not work.

> **P16/L471:** It is not constant due to the variable nature of $Q_t$? If so, explicitly say so.

The time variability of $Q_t$ is not the only reason. In the simulations from Sections 3.1 and 3.2, the effect (intra-storm time-varying concentrations $c(e), c-1(e+1), c-2(e+2)$) does not occur or only to a small extent.

> **P18/Conclusions:** The limitations of current model need to be briefly summarized as well.

Yes, I agree.

> **Figure A1:** This figure gave me hard time at the beginning, as it is depicted by forward concept not backward notation, while the latter is dominated the text. Need more information in the caption to explain this so that readers follow it easily.

I agree, the presentation is not that accurate. I should emphasize the backward perspective. It is not necessary to focus so much on the precipitation $J$.

> **Figure A2:** Though this model was explained in the text, enough information should be given in the caption to make it stand by itself. At least parameters (alpha and eta) need to be explained in the caption for better readability.

Yes, I agree.

> **Figure A3:** Missing the second y-axis labels.

There is only y-axis in this figure, but I will improve or remove the tickmarks on the right hand side.
> Figure A4: For one or two curves, why not smoothed near the end? I do not remember if this has been explained in the text.

Near the end the condition numbers are very high (up to $2 \times 10^6$). In line 289, I have mentioned that "there are increasing (numerical) instabilities in the last events".

> Figure A5: Extremely hard to distinguish the curves, which occurs in other figures as well.

Yes, sometimes not that easy to distinguish, you have to zoom in. I will try with wider lines.

> Figure A9: Need to say what the two arrows are for in the caption.

Yes, I agree.

> Figure A15: Where is precipitation? Also, missing mentioning ce (e as subscript) in the caption. The same issue exists for Figure A18.

I agree, and will improve the figures A15 and A18.

Thank you for your help and feedback.

With kind regards,
Simon Hoeg

Additional References: