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Optimal hydrograph separation filter to evaluate transport routines of hydrological models

Alon Rimmer [a,*], Andreas Hartmann [b]

[a] Israel Oceanographic and Limnological Research Ltd., The Yigal Allon Kinneret Limnological Laboratory, P.O.B. 447, Migdal 14950, Israel
[b] Department of Civil Engineering, Queen's School of Engineering, University of Bristol, United Kingdom

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ABSTRACT

Hydrograph separation (HS) using recursive digital filter approaches focuses on trying to distinguish between the rapidly occurring discharge components like surface runoff, and the slowly changing discharge originating from interflow and groundwater. Filter approaches are mathematical procedures, which perform the HS using a set of separation parameters. The first goal of this study is to minimize the subjective influence that a user of the filter technique exerts on the results by the choice of such filter parameters. A simple optimal HS (OHS) technique for the estimation of the separation parameters was introduced, relying on measured stream hydrochemistry. The second goal is to use the OHS parameters to benchmark the performance of process-based hydro-geochemical (HG) models. The new HG routine can be used to quantify the degree of knowledge that the stream flow time series itself contributes to the HG analysis, using newly developed benchmark geochemistry efficiency (BGE). Results of the OHS show that the two HS fractions ("rapid" and "slow") differ according to the HG substances which were selected. The BFI_{max} parameter (long-term ratio of baseflow to total streamflow) ranged from 0.26 to 0.94 for SO_4^{-2} and total suspended solids, TSS, respectively. Then, predictions of SO_4^{-2} transport from a process-based hydrological model were benchmarked with the proposed HG routine, in order to evaluate the significance of the HG routines in the process-based model. This comparison provides valuable quality test that would not be obvious when using the traditional measures like r^2 or the NSE (Nash–Sutcliffe efficiency). The process-based model resulted in $r^2 = 0.65$ and NSE = 0.65, while the benchmark routine results were slightly lower with $r^2 = 0.61$ and NSE = 0.58. However, the comparison between the two model resulted in obvious advantage for the process-based model with BGE = 0.15.

1. Introduction

Classical hydrograph separation (HS) approaches try to distinguish between direct stream flow, occurring shortly after rainfall, and the remaining flow ("baseflow") component, which reaches the stream with considerable delay (Hall, 1968). Traditionally, hydrograph separation was referred to as "baseflow separation" (Hall, 1968; Tallaksen, 1995) which is usually uniquely attributed to the groundwater component of the stream flow. HS was usually applied for the classical differentiation between the rapid surface runoff ("quick flow") and the slowly changing discharge ("baseflow") from interflow and groundwater (Nathan and McMahon, 1990; Padilla et al., 1994; Aksoy et al., 2008; Wittenberg and Sivapalan, 1999). However, recent studies demonstrated that there are multiple justifications for using various HS techniques at varying time scales, and for various purposes.

HS is used to develop catchment management strategies (Smakhtin, 2001), and to study water quality dynamics or the geochemical nature of various contributors to the stream flow (Neff et al., 2005; Wenninger et al., 2008; Tilahun et al., 2013). In some cases these studies are conducted using hydrochemical components (Christophersen and Hooper, 1992; Lee and Krothe, 2001), water isotopes (Klaus and McDonnell, 2013; Sklash and Farvolden, 1979), or both (Brown et al., 1999; Uhlenbrook et al., 2002). Finally, HS was also used for preparation of time series in modeling verification and calibration (Rimmer and Salingar, 2006; Eckhardt, 2008).

The HS techniques can be divided into 3 categories (Lott and Stewart, 2012): analytical, recession curve and digital filters methods. The analytical category contains methods using linear and non-linear reservoir (Aksoy and Wittenberg, 2011). Various recession curve analysis such as "master" and "individual" recessions were reviewed by Tallaksen (1995). The technique, which has been selected for this study (Eckhardt, 2005) uses a recursive digital filter and is based on the linear reservoir assumption. The filter

* Corresponding author. Tel.: +972 4 4909320; fax: +972 4 6724627.
E-mail address: alon@ocean.org.il (A. Rimmer).

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originates from the literature of signal processing. It is designed to separate "high frequency signals" from "low-frequency signals". Nathan and McMahon (1990) pioneered the use of this family of techniques in hydrology, considering daily stream flow time series to be a mixture of quick flow (high-frequency signal) and base flow (low-frequency signal). Smakhtin and Watkins (1997) tested similar method intensively on daily stream flow data, and Hughes et al. (2003) determined regional HS parameters for both daily data and monthly data in 6 South African catchments. The HS variation of Eckhardt (2005) is especially suitable for large streams in the East Mediterranean region, since during the dry season groundwater recharge cease completely, stream flow depends on groundwater storage, and therefore recesses exponentially.

Eckhardt (2005) raised the question of how to minimize the subjective influence that a user of the filter technique exerts on the results by the choice of filter parameters. He claimed that more available data can be helpful, and that the results of tracer experiments and measurements might possibly lead to general recommendations for separation parameters. Recently, several studies used natural tracers to separate the flow into a number of components (Wenninger et al., 2008; Lott and Stewart, 2012). However, these studies did not propose a general HS optimization technique.

During the last decade gradual amount of modeling studies used hydrochemical, or tracer data, to evaluate and improve model structures (Hartmann et al., 2012; Son and Sivapalan, 2007; Weiler and McDonnell, 2004). The optimal OHS parameters can be used to establish a reference simulation, or a "benchmark routine" for stream hydrochemistry. This type of model is an essential tool to evaluate model successes because unlike the traditional measure of performance such as the Nash–Sutcliffe efficiency (NSE), its reference is not only the seasonal average of the observations (regarded as the "the simplest imaginable model" by Schaefli and Gupta, 2007). The proposed routine can either be used to examine whether the hydro-geochemical (HG) routines of a process-based simulation model have greater explanatory power than is already contained in the model driving forces (the stream flow), and whether the more complex structure of a process-based model really contributes for better predictions.

The first goal of this paper is an attempt to meet the challenge of Eckhardt (2005). A simple optimal hydrograph separation technique (OHS) is proposed in order to reach estimations of separation parameters that rely not only on the measured stream flows, but also on different measured aspects of stream hydro-geochemistry. The second goal of the paper is to demonstrate how the OHS parameters can be used in order to evaluate the performance of stream geochemistry modelling. These objectives were achieved in three steps elaborated in the methodology section: a. The OHS development; b. the use of the OHS parameters to create the hydro-geochemical (HG) benchmark routine; and c. the use of the benchmark routine to test the performance of geochemistry models.

2. Methodology

2.1. Optimal hydrograph separation

2.1.1. The algorithm

The proposed algorithm is based on two types of observed time series. The first is the flow hydrograph $Q(t)$. This time series is usually continuous and typically the basic data set to separate systematically the fast and slow discharge components. The second type (with the general name C_{obs}) is an additional time series which can include occasional observations of HG measurements, such as natural tracer (e.g. Cl^- or SO_4^{-2}); sediments concentration (e.g. TSS, turbidity); and/or nutrients (e.g. NO_3). Being more expensive and discrete by nature, these measurements are usually sporadic, or at best, taken with much longer time intervals then the stream flow measurements (Lott and Stewart, 2012).

The optimization of the HS is conducted according to the following steps (Fig. 1): (1) The measured stream flow time series $Q(t)$ is separated into two components ($Q_B(t)$ and $Q_S(t)$) using an initial combination of the two parameters, α and β, that control the separation process (see theory section and Eckhardt, 2005). (2) The concentration of the specified geochemical tracer for each of the two flow components (C_B and C_S) is assessed. (3) A simple mixing calculation is performed, to create a continuous time series $C_{sep}(t)$ of stream flow concentration. (4) The speculated stream flow concentration is compared to the measured data C_{obs}, and the error of the approximated values is evaluated. Finally, in step 5 the process 1–4 repeats with different separation parameters until a minimal error is reached. The complete procedure is described in the following sections.

2.1.2. Theory – hydrograph separation using recursive digital filter

In the HS filter that was used, the Eckhardt (2005) method, stream flow is described by:

$$Q_j = Q_{B_j} + Q_{S_j} \tag{1}$$

where Q is the total measured streamflow, Q_S the fast occurring quick flows, Q_B is the low-frequency base flow, and j the daily time step number. For clarity the definitions of "base flow" for Q_B and "fast flow" for Q_S will remain throughout the paper.

Using the measured discharge Q_j, the previously $(j-1)$ calculated base flow Q_{Bj-1}, and two filter parameters α and β (same as BFI_{max}, the maximum value of the baseflow index in Eckhardt, 2005) the base flow component Q_{Bj} of time step j is calculated:

$$Q_{B_j} = \frac{[(1-\beta)\alpha Q_{B_{j-1}} + (1-\alpha)\beta Q_j]}{(1-\alpha\beta)}; \quad \begin{array}{c} Q_{B_j} \leqslant Q_j \\ 1 >= \beta >= 0 \end{array}. \tag{2}$$

In the special case when $\beta = 0$, the filter parameter α corresponds to the recession constant in the equation:

$$Q_{B_j} = \alpha Q_{B_{j-1}} \tag{3}$$

mostly used to describe the linear base flow recession in periods without groundwater recharge. With the data collected during these periods, α can be derived by a recession curve analysis of the hydrograph alone (see section "The α parameter" below). However, the second parameter, β, is a non-measurable parameter. Eckhardt (2005) attempted to find typical β values for classes of catchments in order to minimize the subjective influence that a user of the filter technique exerts on the results by his choice of β. His proposed values were $\beta \cong 0.80$ for perennial streams with porous aquifers, $\beta \cong 0.50$ for ephemeral streams with porous aquifers, and $\beta \cong 0.25$ for perennial streams with hard rock aquifers. Nevertheless, he claimed that an optimization according to the results of newer approaches, e.g., of tracer experiments, would possibly lead to improved recommendations for β (*see* section "The β parameter" below).

2.1.3. The α parameter

During seasons without groundwater recharge (e.g. dry season in Mediterranean regions), stream flow may recess exponentially (Maillet, 1905). During the recession period the daily stream flow Q usually follow the form:

$$Q_j = Q_0 \exp[-k(t_j - t_0)] \tag{4}$$

where t_j is the time (day), Q_0 the stream flow ($m^3\ day^{-1}$) on the first day of the dry period, t_0, and k is the recession constant (day^{-1}). The relation between the filter parameter α (Eqs. (2) and (3)) and the exponential recession constant k is $\alpha = \exp[-k]$.