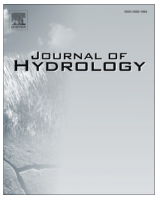
Journal of Hydrology 543 (2016) 59–66

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol



Constitution of a catchment virtual observatory for sharing flow and transport models outputs

Zahra Thomas [a,*], Pauline Rousseau-Gueutin [b], Tamara Kolbe [c,d], Benjamin W. Abbott [d], Jean Marçais [c], Stefan Peiffer [e], Sven Frei [e], Kevin Bishop [f], Pascal Pichelin [a], Gilles Pinay [d], Jean-Raynald de Dreuzy [c]

[a] Agrocampus Ouest, UMR 1069, Soil Agro and hydroSystem, 35000 Rennes, France
[b] EHESP Rennes, Sorbonne Paris Cité, Paris, France
[c] Géosciences Rennes, UMR 6118 CNRS, Université de Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex, France
[d] ECOBIO, OSUR, CNRS, Université de Rennes 1, Campus de Beaulieu, 35042 Rennes, France
[e] Bayreuth Center of Ecology and Environmental Research, Germany
[f] Department of Earth Sciences, Uppsala University, Uppsala, Sweden

ARTICLE INFO

Article history:
Available online 5 May 2016

Keywords:
Transit time distribution
Modelling outputs
Catchment hydrology
Biogeochemistry
Watershed
Inter-catchment comparison

SUMMARY

Predicting hydrological catchment behavior based on measurable (and preferably widely available) catchment characteristics has been one of the main goals of hydrological modelling. Residence time distributions provide synoptic information about catchment functioning and can be useful metrics to predict their behaviors. Moreover, residence time distributions highlight a wide range of characteristic scales (spatial and temporal) and mixing processes. However, catchment-specific heterogeneity means that the link between residence time distributions and catchment characteristics is complex. Investigating this link for a wide range of catchments could reveal the role of topography, geology, land-use, climate and other factors in controlling catchment hydrology. Meaningful comparison is often challenging given the diversity of data and model structures and formats. To address this need, we are introducing a new virtual platform called Catchment virtual Observatory for Sharing flow and transport models outputs (COnSOrT). The goal of COnSOrT is to promote catchment intercomparison by sharing calibrated model outputs. Compiling commensurable results in COnSOrT will help evaluate model performance, quantify inter-catchment controls on hydrology, and identify research gaps and priorities in catchment science. Researchers interested in sharing or using calibrated model results are invited to participate in the virtual observatory. Participants may test post-processing methods on a wide range of catchment environments to evaluate the generality of their findings.

1. Introduction

Predicting hydrological catchment behavior based on measurable (and preferably widely available) catchment characteristics has been one of the main goals of hydrological modelling since the founding of the field over 150 years ago (Mulvany, 1850 in Todini, 2007). Many studies have used topography, geology, land-use, and climate to develop models that can be applied to both gauged and ungauged basins (e.g. Blöschl et al., 2013; Sivapalan, 2003; Soulsby and Tetzlaff, 2008). Technical and theoretical advances in catchment hydrology, including the recent proliferation of commercial and open-source modelling software, have led to a rich diversity of detailed, catchment-specific modelling studies (Beven et al., 2012; Beven and Alcock, 2012; Benettin et al., 2015; Endalamaw et al., 2013; Laudon et al., 2013; Leray et al., 2012; Morton et al., 2014). However, many models have specific, sometimes proprietary data output formats such as MODFLOW, FEFLOW, HydroGeoSphere and other prominent platforms, hindering inter-catchment comparisons and leaving fundamental questions of catchment functioning unanswered. Inter-catchment comparisons remain rare (McGuire et al., 2005; Tetzlaff et al., 2009b), evidence of how challenging it can be to develop general models or approaches applicable for multiple gauged and ungauged catchments.

The mean transit time and whole stream residence time distribution are powerful metrics of catchment functioning, providing synoptic hydrological information such as water renewal time, heterogeneity of flowpaths, and overall water volume (Godsey et al., 2010; Hrachowitz et al., 2010; Marçais et al., 2015;

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* Corresponding author.
E-mail address: zthomas@agrocampus-ouest.fr (Z. Thomas).

http://dx.doi.org/10.1016/j.jhydrol.2016.04.067

McGuire and McDonnell, 2006; Van der Velde et al., 2012). These hydrological parameters influence catchment biogeochemistry (Ocampo et al., 2006; Oldham et al., 2013; Pinay et al., 2015; Tetzlaff et al., 2007), further increasing their value as indicators and predictors of catchment-scale water quality and chemistry. Because these parameters are of great general interest they feature prominently in the inputs and outputs of many models (e.g. McGuire et al., 2005; Tetzlaff et al., 2009a). In combination with generic model results such as flow lines or path lines, residence time distributions represent a potential tool to compare a wide variety of models and model types from different climatic, topographic and hydrogeological contexts. Such tools may help to bring out general approaches for inter-catchment comparison.

To facilitate the comparison and improvement of hydrological models and general understanding of hydrological behavior at the catchment scale, we have created a working group and repository for researchers to share metadata and calibrated model outputs. This virtual observatory called Catchment virtual Observatory for Sharing flow and transport models outputs (COnSOrT) provides a platform to compare catchment response and to extensively test modelling approaches (frameworks, post-processing, lumped, etc.). Our main objective is to collect model outputs from small catchments in differing geological and hydrological conditions to identify controls on biogeochemical and hydrologic functioning in a standardized way that allows direct comparison of model out puts. We are proposing that RTDs and their parameterization are a global platform to characterize and compare catchments. To these ends we are proposing to establish a virtual observatory that will allow testing of research questions that are difficult to address individually including: (i) How do topography and geomorphology influence hydrology across catchments, (ii) What modelling concepts and approaches perform best across catchments, and (iii) What are the relevant metrics of catchment vulnerability in regards to contaminant transport or removal for different degrees of anthropogenic disturbance? Below we outline the initial rationale for COnSOrT, describe the general data structure, and give an example showing how outputs from different modelling platforms can be synthesized.

2. Time distributions as a comparable metric of catchment hydrology

2.1. Starting with small catchments and groundwater flow cells

While the ultimate goal of COnSOrT and catchment hydrology in general is to understand the mechanisms regulating hydrological functioning across spatiotemporal scales, there are several reasons why it makes sense to start small. All waterways, surface or subsurface, start in small catchments. Headwater catchments are typically defined as watersheds smaller than 100 km^2, though this definition is strictly operational and cut-offs ranging from 0.1 km^2 to over 100 km^2 can be found in the literature (Buttle, 1998; Maher, 2011; Moldan and Černý, 1994; Tetzlaff et al., 2008). Headwater catchments occupy an influential position in the landscape (Jones et al., 2005), they are a major component of controlling groundwater recharge and overall water residence time (Alexander et al., 2007), and they make up the bulk of global lotic ecosystems, with 90% of stream length occurring in catchments smaller than 15 km^2 (Bishop et al., 2008). Small catchments express a wide diversity of subsurface flow configurations (Eberts et al., 2012; Gburek and Folmar, 1999; Sophocleous, 2002; Winter, 1999) depending on geological and topographical structures, distribution and timing of recharge, characteristics of the vadose zone, and free surface dynamics of the underlying aquifer (Bresciani et al., 2014; Schumann et al., 2010; Freer et al., 2002; Montgomery and Dietrich, 1989; O'loughlin, 1981; Šimůnek et al., 2003; Voeckler et al., 2014; Dages et al., 2009; de Vries and Simmers, 2002; Scanlon et al., 2002).

Perhaps most importantly in regards to catchment hydrology, small catchments are a convenient and powerful experimental unit. Compared to large catchments, there are fewer processes influencing behavior of small catchments and collecting detailed biogeochemical and hydrological data is more feasible at a small scale. It is also easier to find multiple, nearby catchments with similar climate and environmental contexts, or conversely catchments with distinct characteristics such as fertilization, harvest, or natural disturbance regimes, allowing the identification of controls on catchment functioning. While the great diversity of small catchment behavior complicates predictions for ungauged catchments and the regionalization of models based on well-monitored sites (Hrachowitz et al., 2013; Schilling et al., 2013; Tetzlaff et al., 2010), it emphasizes the importance of inter-catchment comparisons to validate model operation and to remove site-specific relationships. Substantial unknowns persist about the functioning of small catchments, representing a major gap in our understanding of hydrological and biogeochemical functioning of coupled aquatic and terrestrial ecosystems (Bishop et al., 2008; Cole et al., 2007). The growing abundance of small catchment studies in multiple biomes and ecosystem represents an opportunity to address these uncertainties (Benettin et al., 2015; Bormann and Likens, 1994; Jones et al., 2005; Laudon et al., 2011; Likens, 2013; Swank and Crossley, 1988).

Understanding the organization of groundwater flows has been in the center of many researches. Tóth (1963) developed a conceptual model in which under a hummocky water table, groundwater flows are distributed into local, sub-local and regional flows. Numerous studies have used this theory (e.g. Cardenas, 2007; Goderniaux et al., 2013) in order to understand groundwater flows at the regional scale (nested catchment scale). Those studies emphasize the relation between the topography and the geology to control the regional, sub-local and local flows (e.g., Haitjema and Mitchell-Bruker, 2005; Freeze and Witherspoon, 1967). The time distribution has been used in those regional studies in order to identify relationship between the time distribution and the nested flow organization (Kolbe et al., 2016; Eberts et al., 2012).

2.2. Time distribution terms and concepts

The amount of time water remains in a catchment is one of the key parameters controlling biogeochemical functioning and can vary in small catchments from a few days to millennia (McDonnell and Beven, 2014; Moldan and Černý, 1994; Rodhe et al., 1996; Frisbee et al., 2013). The mean transit time, or the average amount of time a water molecule stays within the watershed boundaries, is an integrated measure of catchment residence time (e.g. Capell et al., 2012; McGuire et al., 2002; Soulsby and Tetzlaff, 2008). Transit and residence times are two common metrics of how long water stays in a system. Transit time is defined as the time that water takes to reach the outlet of a system, whereas the residence time is the time since water entered the system calculated at any sampling location of interest (McGuire and McDonnell, 2006). Because these measures are analogous for our purposes, we will hereafter refer to their distributions as travel time distributions. The realization that catchment travel time distributions are usually very skewed with long tails (Kirchner et al., 2001) has focused recent analysis on the whole travel time distribution (Dunn et al., 2010).

As it is impractical to measure the whole travel time distribution using injected hydrological tracers (but see Rodhe et al., 1996), different approaches, such as lumped parameter models, particle-tracking, and direct age simulation, have been developed to estimate travel time distributions (Turnadge and Smerdon,