CIVE 625 – Quantitative Ecohydrology

Lab 4 – (Due Date: May 8th)

Introduction the StorAge Selection (SAS) Framework

Background

Understanding the dynamics of catchment hydrology is crucial for effective water resources management, particularly in light of environmental changes. A key component in modern hydrological modeling is transit time—the duration water spends traveling through a catchment from input to output. The StorAge Selection (SAS) framework has emerged as a significant tool to explore these dynamics, modeling how water and the solutes it carries move through a catchment based on the age of the water.

Additionally, this framework allows us to examine how vegetation activity through evapotranspiration can alter water and solute fluxes at a catchment's outlet. This lab uses the dataset from the Lower Hafren watershed in Wales shown in Kirchner (2003).

Objectives

This lab is designed to deepen our understanding of the SAS framework by applying it to progressively complex scenarios. You will explore how the water age balance equation responds to different storage selection functions and how these choices affect predicted solute concentrations at a watershed's outlet. Specifically, we will:

Let's recap a bit of theory:

Before we start playing around with water ages, let's review a few concepts.

The ranked storage selection theory (rSAS) is one of the existing variations within the SAS framework (Benettin et al., 2022). In this theory, the system is assumed to be a single control volume, subject to a precipitation $J(t)$ input flux and the output fluxes from discharge $Q(t)$ and evapotranspiration $ET(t)$.

At any moment t, the ages ($\mathcal{T}$) of water in storage can be represented by the residence time distribution $P_S(T,t)$, representing the cumulative distribution of ages within the system. The fluxes in and out of the system will alter the structure of $P_S(T,t)$ over time, through the cumulative backwards transit times distributions (bTTD) of discharge $\overleftarrow{\Omega_Q}(T,t)$ and evapotranspiration $\overleftarrow{\Omega_{ET}}(T,t)$.

The continuity equation for the ages and storage within the system, can be written in a cumulative form as (Harman, 2015)

$$\frac{\partial S_T(T,t)}{\partial t} = J(t) - Q(t)\Omega_{\mathrm{Q}}(S_T,t) - ET(t)\Omega_{\mathrm{ET}}(S_T,t) - \frac{\partial S_T(T,t)}{\partial T}, \quad (1)$$

where the age-ranked storage, $S_T(T,t)$ represents the actual storage having ages $\mathcal{T} < \mathrm{T}$:

$$S_T(T,t) = S(t)P_S(T,t) \quad (2)$$

where $S(t)$ represents storage, in mm. Equation 1 shows that S_T is modified in time by the increase in storage from precipitation (assumed to have age equal to zero), the decrease in storage with age selection being determined from $\Omega_Q(T,t)$ and $\Omega_{ET}(T,t)$ and the ageing of water within the system as $\frac{\partial S_T(T,t)}{\partial T}$. The rSAS functions therefore represent the outflux selection from the age-ranked storage.

Lab instructions:

Open the code Lab4.m. The instructions will follow each section of the code:

Part 0:

In Part 0 of the lab, we begin by loading and visualizing data obtained from Kirchner (2003). This dataset includes information on precipitation (P), discharge (Q), and chloride concentration (Cl) in precipitation and discharge. We then proceed to implement a simple hydrologic model to simulate precipitation, discharge, and evapotranspiration (ET) based on the observed data. This allows us to compare the simulated values with the observed ones, providing insight into the performance of the model in replicating real-world hydrological processes.

Take a moment to visualize the observed data in Figure 1 and play around with different observation windows from those given in the code. Note that the hydrologic model used here is an even simpler version of the Toy Model we used at previous labs, and that there are only two parameters: S_{umax}, the catchment-scale storage capacity that is used to scale PET into ET, and K, the recession constant. Play around with values of this simple model to obtain a response that seems reasonable based on hydrograph comparison. You will not find a perfect fit.

- **For this part, plot Figures 1 and 2 and write down your thoughts.**

Part 1: Initial distribution of ages in storage.

Here you will work with the definition of an initial age distribution. You will first define a probability distribution in pdf format. Given an initial storage (in mm) that you will assign, you then plot in Figure 3 the following: (i) the chosen pdf, (ii) the initial age distribution $s_T(T,t=0)$, and finally the initial age ranked storage $S_T(T,t=0)$ (see equation 2). There are 3 options you can chose from to explore this transformation, a normal, exponential and uniform distribution. Explore the different shapes and implications of those choices, along with the choice of an initial volume.

- **For this part, plot Figure 3 and write down your thoughts.**

<u>Part 2: Effect of aging.</u>

Here we will simply observe part of the water ages balance. If we assume there is no water entering or leaving the watershed, equation 2 becomes:

$$\frac{\partial S_T(T,t)}{\partial t} = -\frac{\partial S_T(T,t)}{\partial T} \tag{3}$$

Which means that the only term altering S_T will be the increase in age of the water already in the system. A simple loop is written in which you can explore this isolated effect on S_T. In Figure 5, you will see this effect in terms of the changes in $s_T(T,t)$ and $S_T(T,t)$ and also track the total storage in the system.

- **For this part, plot Figure 4 and write down your thoughts. What is happening here?**

<u>Part 3: Effects of aging and precipitation.</u>

Let's now add one more layer of complexity. We will now assume there is new water being added to the system as precipitation, but no water is leaving (yet!).

$$\frac{\partial S_T(T,t)}{\partial t} = J(t) - \frac{\partial S_T(T,t)}{\partial T} \tag{4}$$

In Figure 5, you will see this effect in terms of the changes in $s_T(T,t)$ and $S_T(T,t)$ and also track the total storage in the system.

- **For this part, plot Figure 5 and write down your thoughts. What is happening here?**

<u>Part 4: Effects of aging, precipitation and storage selection function on discharge.</u>

Let's now consider the water leaving the system as discharge (Q(t)). For that we need to implement the Omega function. The omega function defines a distribution of water ages that will be removed from system, i.e. that will be applied to the $S_T(T,t)$. Our water age-balance equation becomes.

$$\frac{\partial S_T(T,t)}{\partial t} = J(t) - Q(t)\Omega_{\mathrm{Q}}(S_T,t) - \frac{\partial S_T(T,t)}{\partial T} \tag{5}$$

In Figure 6, you will see this effect in terms of the changes in $s_T(T,t)$ and $S_T(T,t)$ and also track the total storage in the system. You will have two options for defining Ω_{Q}, as a gamma distribution and as an exponential distribution. Note that for the gamma option two inputs are needed: mean and variance, while for the exponential option you only need to define one parameter, the mean (the exponential is an easier choice).

- **First by plotting an example for one of the distributions, what the choice of the mean values, for gamma, or mean values, for exponential mean in terms of the ages of water that will be predominantly sampled from S_T.**
- **As before, for this part, plot Figure 6 and write down your thoughts. What is happening here for each subplot.**

Part 5: Effects of aging, precipitation and storage selection functions on Q and ET

We will now consider the water leaving the system as both discharge (Q(t)) and ET(t). For that we need to implement the Omega function for ET:

$$\frac{\partial S_T(T,t)}{\partial t} = J(t) - Q(t)\Omega_{\mathrm{Q}}(S_T,t) - ET(t)\Omega_{\mathrm{ET}}(S_T,t) - \frac{\partial S_T(T,t)}{\partial T} \tag{5}$$

In Figure 7, you will see this effect in terms of the changes in $s_T(T,t)$ and $S_T(T,t)$ and also track the total storage in the system. The code let's you model Ω_{ET} through a uniform distribution function with pre-defined bounds. Feel free to change the range of ages to be sampled by vegetation (defined by a and b in the code).

- **Plot your choice of Ω_{ET}, and write down your thoughts as to what those choices mean in practice.**
- **For this part, plot Figure 7 and write down your thoughts. What is happening here?**

Part 6: Capturing catchment-scale solute concentration responses.

Assuming a given concentration of a conservative tracer in the rainfall is known, the age-water balance equation allows us to calculate the concentration of that given tracer in the outputs (streamflow and/or ET). Our example dataset uses Chloride measured in the rainfall as the conservative tracer in question. We will now compute the chloride concentration in the outflows obtained by following the SAS functions we defined previously.

Chloride can be assumed to be conservative for streamflow, but not for ET (plants regulate the concentration of salts as part of their mechanisms for moving water by controlling water potentials within the plant). Ideally, we would need to sample other tracers such as naturally occurring water isotopes in the rain (^{2}H and ^{18}O) and in the plant tissue to make this type of analysis with real world data. However, for our example let's assume that Chloride will pass through plants without problems.

The code in Part 6 uses the pdf of the Ω_Q and Ω_{ET} (ω_Q and ω_{ET}) to compute the tracer concentration at water leaving the watershed as both Q and ET. This can be done because the ω functions inform the amount of water selected to leave the watershed for a range of ages. If we know the tracer concentration of rainfall, we can simply use those concentration values to "label" water entering the system at different time steps.

For example, let's say that at a given timestep "t", the discharge is equal to 10mm. Additionally, the ω_Q value for water with age = 50 days is 0.7mm:

$$Q(t) \times \omega_{\mathrm{Q}}(T = 50, t) = 0.7 \tag{6}$$

This means that the outflow for that given day will have 0.7 mm of water having 50 days. The concentration of chloride of water having 50 days is the concentration of chloride of the rainfall that fell 50 days prior to the timestep "t". Finally, at the timestep "t" the total concentration of chloride in the discharge can be calculated as a weighted sum of the discharge fractions of water having different ages multiplied by the corresponding chloride concentrations for those ages.

After running Part 6 of the code, you will obtain Figure 8. Here, you can see the Chloride concentrations at both discharge and ET, simulated by our SAS model, and also, as previously shown, the chloride concentrations at rainfall and discharge, measured at the given site.

- **Who has a "flashier" response, ET or Q? Why?**
- **How would the choice of your SAS functions change the outputs you see here: Repeat this Figure 8 by modifying the SAS function for Q and ET and explore the sensitivity of the results.**

Part 7: Time Variable SAS function (OPTIONAL).

In this part you will be able to set a range of values for the mean age in Ω_Q to be an inverse function of storage in the system. This will imply that when storage is high, lower means will be applied to the distribution of ages of water sampled to become discharged, while higher means will be applied when storage is low.

- **Adjust the range accordingly and discuss if that modification resulted in better representation of chloride at the discharge values.**

REFERENCES:

Kirchner, J. W. (2003). A double paradox in catchment hydrology and geochemistry. *Hydrological Processes, 17*(4), 871-874. https://doi.org/10.1002/hyp.5108

Benettin, P., Rodriguez, N. B., Sprenger, M., Kim, M., Klaus, J., Harman, C. J., et al. (2022). Transit time estimation in catchments: Recent developments and future directions. Water Resources Research, 58, e2022WR033096. https://doi.org/10.1029/2022WR033096