Simple one-dimensional tool to simulate solute transport in river as a binary mixture of fast and slow components

Supplementary material to **hydrology-2718671** "*The potential of isotopic tracers for precise and environmentally clean stream discharge measurements*" submitted by Picard et al.

Mathematical background of the model

A binary 1-D dispersion model to simulate artificial tracer injections in river has been developed. It allows to determine flow parameters such as dispersion, velocity and the influence of slower velocity zones. A similar lumped parameter model approach was used to simulate the transport of an artificial tracer release in the Rhine river and is described in Leibundgut et al [1].

Assuming a conservative tracer, with no background concentration, the classical 1-D lumped dispersion model can be expressed under the following form [2]:

$$C(t)=\int_{-\infty}^{t} C_{inj}(\tau)g(t-\tau)\,d\tau \qquad \text{(S1)}$$

Where:

$$g(\tau)=\frac{v}{x\sqrt{4\pi\frac{D}{x^2}\tau}}\,e^{\frac{\left(1-\frac{\tau v}{x}\right)^2}{4\tau\frac{D}{x^2}}} \qquad \text{(S2)}$$

With C being the tracer concentration over time [ML^{-3}], D being the longitudinal dispersion parameter [L^2T^{-1}], x the distance between the injection and measurement points [L] and v the mean stream velocity [LT^{-1}]. C_{inj} is the injection function [ML^{-3}]. It consists of a Dirac-type function in the case of an instantaneous injection, but any kind of injection scheme can be modelled using this tool.

In this binary mixing model approach, the measured tracer concentration was simulated by adding a second flow component representing the slower fraction:

$$C(t)=f_1\int_{-\infty}^{t} C_{inj}(\tau)g_1(t-\tau)\,d\tau+(1-f_1)\int_{-\infty}^{t} C_{inj}(\tau)g_2(t-\tau)\,dt \qquad \text{(S3)}$$

Use of the model

The model consists of six sheets. They are described below.

1- *Description of DM_fast, DM_slow and BMM_DM_DM and GRAPHS_TRACER*

The Eq. (S3) consists of two integrals that are separately solved in DM_fast and DM_slow using the classical trapezoidal integration scheme. Mass conservation is verified by computing the total tracer recovery. The sheet BMM_DM_DM uses the results in DM_fast and DM_slow to simulate the total flow using the parameter f_1 (see column H). Results are plotted in the sheet GRAPHS_TRACER.

The user shouldn't modify any cell of all these sheets.

2- Description of Field data

The user is invited to enter data from the field in this sheet (see column C):

- Time step of calculation: expressed in seconds, has to be at least 1 s. It should be optimized according to the duration of the experiment.
- Section length: is the longitudinal distance between the injection point and the restitution point
- Tracer concentration before injection: expressed in mol/L, is the background concentration of the tracer
- Discharge: it is automatically calculated using field data pasted in column G
- Tracer used: simply put the name of the tracer used
- Duration of injection: expressed in seconds, should be at least 1s if the injection is instantaneous. Any duration can theoretically be modelled
- Moles of tracer injected: simply put the number of moles injected
- Tracer molar mass: expressed in g/mol, is the molar mass of the tracer that is injected
- Columns F and G: this is tracer field data (in the example, you can find discrete analyses of deuterium concentrations over time)

The parameters of the model can be fitted in this sheet by using the Excel Solver. The mean square root deviation (calculated in cell B13) has to be minimized by optimizing parameters D, v and f_1 in cells B17, B18, B19, C17 and C18 (see blue cells). These are the river flow transport parameters (dispersion, velocity) and the partition between the fast and slower components (f_1). In the provided deuterium example, $D_1 = 0.12$ m²/s, $v_1 = 0.10$ m/s, $D_2 = 0.22$ m²/s, $v_2 = 0.07$ m/s and $f_1 = 0.57$.

3- Description of 2H_37Cl_constants

This sheet consists of useful constants for isotopic tracers. In addition, a "note to users" and calculations for ^{37}Cl are provided. Indeed, isotopes results from the laboratory are usually reported in δ-values. This is not convenient for this model, as it requires tracer concentrations expressed in mol/L. Calculations details for ^{37}Cl are provided as it is not an easy task to convert δ-values to $mol_{^{37}Cl}$/L.

The $\delta^{37}Cl$ of the river before injection and the total chloride concentration must be provided by the user in cells B14 and B15 respectively. This allows to compute the ^{37}Cl concentration naturally present in the river before injection. The $\delta^{37}Cl$ of the injected salt as well as the mass of chloride injected must be provided by the user in cells B22 and B23. This is useful to compute the exact quantity of ^{37}Cl injected (cell B28). The "note to users" provides additional details regarding the use of these information (copy/paste values in other sheets if needed etc.).

References

1. Leibundgut, C., P. Maloszewski, and C. Külls, *Tracers in Hydrology*. 2009: Wiley-Blackwell.

2. Jurgens, B.C., J.K. Böhlke, and S.M. Eberts, *TracerLPM (Version 1): An Excel Workbook for interpreting groundwater age distributions from environmental tracer data*, ed. USGS. 2012. 72.