ADVANCING EARTH AND SPACE SCIENCE

Water Resources Research

COMMENTARY
10.1029/2022WR031987

Addendum to "Quantifying Uncertainty in Tracer-Based Hydrograph Separations" for Three-Component Mixing Problems

David P. Genereux[1]

[1]Department of Marine, Earth, and Atmospheric Sciences, North Carolina State University, Raleigh, NC, USA

Key Points:

- A widely cited 1998 paper on uncertainty analysis for water mixing problems does not present critical equations for three-component problems
- The equations are presented here to facilitate calculation of uncertainty in three-component mixing problems

Correspondence to:
D. P. Genereux,
genereux@ncsu.edu

Citation:
Genereux, D. P. (2022). Addendum to "quantifying uncertainty in tracer-based hydrograph separations" for three-component mixing problems. *Water Resources Research*, *58*, e2022WR031987. https://doi.org/10.1029/2022WR031987

Received 12 JAN 2022
Accepted 3 FEB 2022

Author Contributions:
Conceptualization: David P. Genereux
Formal analysis: David P. Genereux
Funding acquisition: David P. Genereux
Investigation: David P. Genereux
Methodology: David P. Genereux
Writing – original draft: David P. Genereux
Writing – review & editing: David P. Genereux

Abstract Water mixing problems are common in hydrology. A 1998 paper describing uncertainty analysis in tracer-based mixing problems is widely cited but does not present the equations needed for three-component problems. This Commentary presents the equations needed to compute the uncertainties in the mixing fractions for a three-component water mixing problem based on tracer data.

1. Commentary

Water mixing problems have long been studied in hydrology, and Genereux (1998) presents an approach that is widely used to estimate uncertainty when chemical or isotopic tracers are used to quantify the mixing of two different waters or "components" (e.g., Boithias et al., 2021; Fillo et al., 2021; Maier & van Meerveld, 2021; Miller et al., 2021; Saiers et al., 2021; Zhou et al., 2021). In such two-component cases, Equations 1 and 2 in Genereux (1998) are used to compute the mixing fractions f_1 and f_2 (i.e., the proportions of components 1 and 2 in the mixture), and Equation 4 is used to compute the uncertainty in the mixing fractions.

Genereux (1998) describes how equations analogous to Equation 4 could be derived for uncertainty analysis of three-component water mixing problems, and shows results from applying those equations to a three-component example problem, but does not explicitly present the full set of equations needed. This represents an important gap for researchers needing to compute the uncertainties in mixing fractions for three-component problems.

This commentary fills that gap by providing the equations needed for uncertainty analysis in situations involving mixing of three different waters.

For a mixture of three components, Equations 8–10 in Genereux (1998) are used to compute the mixing fractions (f_1, f_2, and f_3) from eight tracer concentrations: the concentrations of two different tracers in four different waters (the three components and the mixture of the components). Quantifying the uncertainties in the mixing fractions requires evaluating the partial derivative of each mixing fraction with respect to the eight tracer concentrations. The 24 partial derivatives would be used in Equation 3 in Genereux (1998) to yield the equations needed to compute the uncertainties in f_1, f_2, and f_3, as shown below.

Following notation in Section 4 of Genereux (1998), A and B are the concentrations of the two tracers needed to solve a three-component mixing problem, and subscripts 1, 2, 3, and S indicate the three components and the stream water, the latter being the mixture of the three components. Four variables useful in simplifying the presentation can be defined from the eight tracer concentrations:

$$M_1 = A_S B_2 - A_S B_3 + A_2 B_3 - A_2 B_S + A_3 B_S - A_3 B_2 \tag{1}$$

$$M_2 = A_S B_3 - A_S B_1 + A_1 B_S - A_1 B_3 + A_3 B_1 - A_3 B_S \tag{2}$$

$$M_3 = A_S B_1 - A_S B_2 + A_1 B_2 - A_1 B_S + A_2 B_S - A_2 B_1 \tag{3}$$

$$M_4 = A_1 B_2 - A_1 B_3 + A_2 B_3 - A_2 B_1 + A_3 B_1 - A_3 B_2 \tag{4}$$

M_1 to M_3 are the numerators of Equations 8–10, respectively, in Genereux (1998), and M_4 is the denominator in those same equations.

The 24 partial derivatives of Equations 8–10 in Genereux (1998) are:

$$\frac{\partial f_1}{\partial A_S} = \frac{B_2 - B_3}{M_4} \tag{5}$$

$$\frac{\partial f_1}{\partial A_1} = \frac{-M_1(B_2 - B_3)}{M_4^2} \tag{6}$$

$$\frac{\partial f_1}{\partial A_2} = \frac{M_4(B_3 - B_S) - M_1(B_3 - B_1)}{M_4^2} \tag{7}$$

$$\frac{\partial f_1}{\partial A_3} = \frac{M_4(B_S - B_2) - M_1(B_1 - B_2)}{M_4^2} \tag{8}$$

$$\frac{\partial f_1}{\partial B_S} = \frac{A_3 - A_2}{M_4} \tag{9}$$

$$\frac{\partial f_1}{\partial B_1} = \frac{-M_1(A_3 - A_2)}{M_4^2} \tag{10}$$

$$\frac{\partial f_1}{\partial B_2} = \frac{M_4(A_S - A_3) - M_1(A_1 - A_3)}{M_4^2} \tag{11}$$

$$\frac{\partial f_1}{\partial B_3} = \frac{M_4(A_2 - A_S) - M_1(A_2 - A_1)}{M_4^2} \tag{12}$$

$$\frac{\partial f_2}{\partial A_S} = \frac{B_3 - B_1}{M_4} \tag{13}$$

$$\frac{\partial f_2}{\partial A_1} = \frac{M_4(B_S - B_3) - M_2(B_2 - B_3)}{M_4^2} \tag{14}$$

$$\frac{\partial f_2}{\partial A_2} = \frac{-M_2(B_3 - B_1)}{M_4^2} \tag{15}$$

$$\frac{\partial f_2}{\partial A_3} = \frac{M_4(B_1 - B_S) - M_2(B_1 - B_2)}{M_4^2} \tag{16}$$

$$\frac{\partial f_2}{\partial B_S} = \frac{A_1 - A_3}{M_4} \tag{17}$$

$$\frac{\partial f_2}{\partial B_1} = \frac{M_4(A_3 - A_S) - M_2(A_3 - A_2)}{M_4^2} \tag{18}$$

$$\frac{\partial f_2}{\partial B_2} = \frac{-M_2(A_1 - A_3)}{M_4^2} \tag{19}$$

$$\frac{\partial f_2}{\partial B_3} = \frac{M_4(A_S - A_1) - M_2(A_2 - A_1)}{M_4^2} \tag{20}$$

$$\frac{\partial f_3}{\partial A_S} = \frac{B_1 - B_2}{M_4} \tag{21}$$

$$\frac{\partial f_3}{\partial A_1} = \frac{M_4(B_2 - B_S) - M_3(B_2 - B_3)}{M_4^2} \tag{22}$$

$$\frac{\partial f_3}{\partial A_2} = \frac{M_4(B_S - B_1) - M_3(B_3 - B_1)}{M_4^2} \tag{23}$$

$$\frac{\partial f_3}{\partial A_3} = \frac{-M_3 (B_1 - B_2)}{M_4^2} \tag{24}$$

$$\frac{\partial f_3}{\partial B_S} = \frac{A_2 - A_1}{M_4} \tag{25}$$

$$\frac{\partial f_3}{\partial B_1} = \frac{M_4 (A_S - A_2) - M_3 (A_3 - A_2)}{M_4^2} \tag{26}$$

$$\frac{\partial f_3}{\partial B_2} = \frac{M_4 (A_1 - A_S) - M_3 (A_1 - A_3)}{M_4^2} \tag{27}$$

$$\frac{\partial f_3}{\partial B_3} = \frac{-M_3 (A_2 - A_1)}{M_4^2} \tag{28}$$

Finally, substitution of Equations 5–28 above into Equation 3 in Genereux (1998) gives the three equations needed to compute the uncertainties in the three mixing fractions (one equation for each mixing fraction):

$$W_{f_1} = \sqrt{\left(E_5 W_{A_S}\right)^2 + \left(E_6 W_{A_1}\right)^2 + \left(E_7 W_{A_2}\right)^2 + \left(E_8 W_{A_3}\right)^2 + \left(E_9 W_{B_S}\right)^2 + \left(E_{10} W_{B_1}\right)^2 + \left(E_{11} W_{B_2}\right)^2 + \left(E_{12} W_{B_3}\right)^2} \tag{29}$$

$$W_{f_2} = \sqrt{\left(E_{13} W_{A_S}\right)^2 + \left(E_{14} W_{A_1}\right)^2 + \left(E_{15} W_{A_2}\right)^2 + \left(E_{16} W_{A_3}\right)^2 + \left(E_{17} W_{B_S}\right)^2 + \left(E_{18} W_{B_1}\right)^2 + \left(E_{19} W_{B_2}\right)^2 + \left(E_{20} W_{B_3}\right)^2} \tag{30}$$

$$W_{f_3} = \sqrt{\left(E_{21} W_{A_S}\right)^2 + \left(E_{22} W_{A_1}\right)^2 + \left(E_{23} W_{A_2}\right)^2 + \left(E_{24} W_{A_3}\right)^2 + \left(E_{25} W_{B_S}\right)^2 + \left(E_{26} W_{B_1}\right)^2 + \left(E_{27} W_{B_2}\right)^2 + \left(E_{28} W_{B_3}\right)^2} \tag{31}$$

where W_Y refers to the uncertainty in parameter Y (e.g., W_{f_1} = uncertainty in f_1) and E_x refers to the right-hand side of Equation x above (e.g., $E_5 = (B_2 - B_3) / M_4$). Equations 29–31 above are readily evaluated with data for the eight tracer concentrations needed to solve a three-component mixing problem; results of this for a stream water sample from Virginia are presented in Table 4 of Genereux (1998).

Acknowledgments

The author gratefully acknowledges colleagues who motivated this commentary by requesting information about the equations needed for the three-component case. This work was supported in part by the US National Science Foundation (EAR 1744714).

References

Boithias, L., Ribolzi, O., Lacombe, G., Thammahacksa, C., Silvera, N., Latsachack, K., et al. (2021). Quantifying the effect of overland flow on *Escherichia coli* pulses during floods: Use of a tracer-based approach in an erosion-prone tropical catchment. *Journal of Hydrology*, *594*, 125935. https://doi.org/10.1016/j.jhydrol.2020.125935

Fillo, N. K., Bhaskar, A. S., & Jefferson, A. J. (2021). Lawn irrigation contributions to semi-arid urban baseflow based on water-stable isotopes. *Water Resources Research*, *57*, e2020WR028777. https://doi.org/10.1029/2020wr028777

Genereux, D. P. (1998). Quantifying uncertainty in tracer-based hydrograph separations. *Water Resources Research*, *34*(4), 915–919. https://doi.org/10.1029/98wr00010

Maier, F., & van Meerveld, I. (2021). Long-term changes in runoff generation mechanisms for two proglacial areas in the Swiss Alps I: Overland flow. *Water Resources Research*, *57*, e2021WR030221. https://doi.org/10.1029/2021wr030221

Miller, S. A., Mercer, J. J., Lyon, S. W., Williams, D. G., & Miller, S. N. (2021). Stable isotopes of water and specific conductance reveal complimentary information on streamflow generation in snowmelt-dominated, seasonally arid watersheds. *Journal of Hydrology*, *596*, 126075. https://doi.org/10.1016/j.jhydrol.2021.126075

Saiers, J. E., Fair, J. H., Shanley, J. B., Hosen, J., Matt, S., Ryan, K. A., & Raymond, P. A. (2021). Evaluating streamwater dissolved organic carbon dynamics in context of variable flowpath contributions with a tracer-based mixing model. *Water Resources Research*, *57*, e2021WR030529. https://doi.org/10.1029/2021wr030529

Zhou, J., Ding, Y., Wu, J., Liu, F., & Wang, S. (2021). Streamflow generation in semi-arid, glacier-covered, montane catchments in the upper Shule River, Qilian Mountains, northeastern Tibetan plateau. *Hydrological Processes*, *35*, e14276. https://doi.org/10.1002/hyp.14276