Consistency of Modeled River Tracer Test Breakthrough Curve Moments With Data.

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Abstract

Precise modeling of surface water quality requires transport theory consistent with observed data. Efforts to achieve model fits to river tracer test breakthrough curves (BTCs) have led to different approaches to the one-dimensional modeling of river corridor transport at the macroscale. The memory function model form practically generalizes most current approaches including the transient storage (TSM), multirate mass transfer, decoupled continuous time random walk, and time-fractional advection dispersion models. An alternative formulation of the memory function approach is the phase exposure-dependent exchange (PhEDEx) model, which is the TSM model that includes residence-time dependence of the rate coefficient for mass exchange from the hyporheic zone to the river. Using temporal moment analysis and numerical simulations, we explore the general consistency of the PhEDEx model with observed BTC data. With this approach the moments of the memory function can be estimated without requiring any prior information about the memory function form. We also examine means of estimating river/transport process parameters using the results of temporal moments analysis. The results show the failure of the PhEDEx model, and therefore the memory function approach, in capturing in particular the observed constancy of the BTC coefficient of skewness (CSK). The temporal moments equations can be applied as a useful tool to estimate some river/tracer test parameters such as the ratio of HZ cross-sectional area to the main flow cross-sectional area, which are time/cost consuming to measure. The applications of the analyses are demonstrated with some case studies.

Consistency of Modeled vs. Observed Scaling of Temporal Moments of River Tracer Test Breakthrough Curves.

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Motivation:

All previous 1-D river corridor models predict a CSK that drops with transport distance (~x-1/2) while the data all show a constant CSK[1]. Therefore, there is a need to revise the theory of solute transport to be consistent with the data set.

Research Question:

Is residence time in the hyporheic zone a good representative variable for river corridor transport that can give a constant CSK?

Material and Methods:

PhEDEx[2] = Memory Function

$$\frac{\partial c}{\partial t}+v\frac{\partial c}{\partial x}-D\frac{\partial^2 c}{\partial x^2}=-\beta\left[k_f c-\int_0^t k_r(\omega)s(x,t,\omega)d\omega\right]$$

$$\frac{\partial s}{\partial t}+\frac{\partial s}{\partial \omega}=-k_r(\omega)s \qquad c=c(x,t) \qquad s=s(x,t,\omega)$$

Moments Analysis:

$\mu_n(x)\equiv\int_0^\infty \tau^n C\,d\tau = n^{th}$ moments of BTC

$m_1=\mu_1/\mu_0$ = mean

$m_2=(\mu_2/\mu_0)-(\mu_1/\mu_0)^2$ = variance

$m_3=(\mu_3/\mu_0)-3(\mu_1/\mu_0)(\mu_2/\mu_0)+2(\mu_1/\mu_0)^3$ = skewness

$$CSK=\frac{m_3}{(m_2)^{\frac{3}{2}}}$$

Numerical Solutions:

Explicit Finite Difference

$$\frac{\partial c}{\partial t}+v\frac{\partial c}{\partial x}-D\frac{\partial^2 c}{\partial x^2}=-\beta\frac{\partial}{\partial t}[g*c]$$

$g_G(t)=\gamma\eta(\gamma t+1)^{-(\eta+1)}$ Gamma-distribution Associated Memory Function

Like all previous 1-D river corridor models, PhEDEx/Memory function deliver temporal moments of BTCs such that $CSK=\frac{m_3}{(m_2)^{\frac{3}{2}}}\sim x^{-1/2}$

But data show CSK ~ constant!

Plain Language Schematic

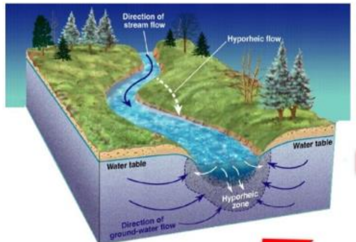
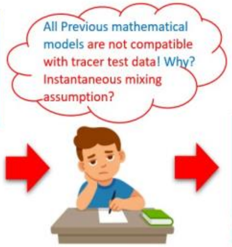


Fig 2. River corridor with groundwater exchange: Transport processes



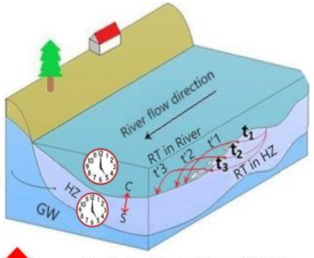


Fig 3. Residence Times (RTs) in Hyporheic Zone and in River can tell us mixing rates !

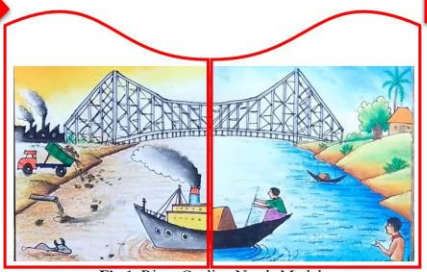


Fig 1. River Cycling Needs Models

Figures adapted from:
Fig.1 www.youtube.com/watch?v=TkTcpqizJFE
Fig.2 . www.waterwired.org/2013/05/from-envagency-the-hyporheic-handbook.html)
Fig.3 web.hku.hk/~maychui/area03.html

Results and Discussions:

Moments Results:

Following the path of Luo et al., (2008)[3]:

$$m_1=A_1\frac{x}{v}+m_1(0)$$

$$m_2=\left(\frac{2A_1{}^2D}{v^2}+A_2\right)\frac{x}{v}+m_2(0)$$

$$m_3=\left(A_3+6\frac{A_1A_2D}{v^2}+12\frac{A_1{}^3D^2}{v^4}\right)\frac{x}{v}+m_3(0)$$

$$m_4=\left(A_4+6A_2m_2(0)+\frac{\left(8A_1A_3D+6A_2{}^2D+12A_1{}^2Dm_2(0)\right)}{v^2}+72\frac{A_1{}^2A_2D^2}{v^4}+120\frac{A_1{}^4D^3}{v^6}\right)\frac{x}{v}+\left(3A_2{}^2+12\frac{A_1{}^2A_2D}{v^2}+12\frac{A_1{}^4D^2}{v^4}\right)\frac{x^2}{v^2}+m_4(0)$$

$$A_1\equiv\beta k_f\int_0^\infty e^{-K(\omega)}\,d\omega+1$$

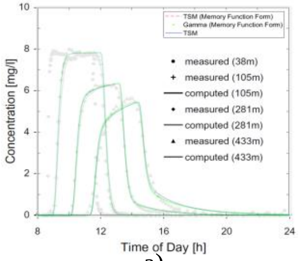
$$A_2\equiv 2\beta k_f\int_0^\infty \omega e^{-K(\omega)}\,d\omega$$

$$A_3\equiv 3\beta k_f\int_0^\infty \omega^2 e^{-K(\omega)}\,d\omega$$

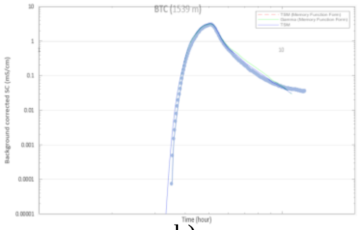
$$A_4\equiv 4\beta k_f\int_0^\infty \omega^3 e^{-K(\omega)}\,d\omega$$

$$K(\omega)\equiv\int_0^\omega k_r(\omega')\,d\omega'$$

Numerical Solutions Results:



a)



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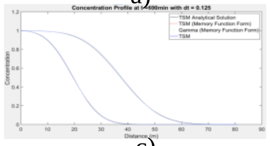

c)

Fig 4. Numerical simulation plots: a) the comparison of Schmid (2003)[4] figure 1 curves with the simulations of TSM and Gamma memory function form, b) the comparison of Sturt river data of McCallum et al., (2020)[5] with the simulations of TSM and Gamma memory function form, c) the comparison of TSM analytical solutions of Lassey (1988), TSM numerical simulations, and numerical simulation for Gamma memory function form for concentration profiles at two different times

Summary and Conclusions:

- All models deliver temporal moments of BTCs such that $CSK=\frac{m_3}{(m_2)^{\frac{3}{2}}}\sim x^{-1/2}$

  But data show CSK ~ constant!
- Like all previous models, PhEDEx/Memory function cannot give a constant or adjustable CSK
- The moments' analysis gives the capability of getting moments of memory function without requiring information about its form.

Citations:

1. González-Pinzón et al.,. (2013). Scaling and predicting solute transport processes in streams. *WRR*, *49*(7), 4071-4088
2. Ginn et al.,. (2017). Phase exposure-dependent exchange. *WRR*, *53*(1), 619-632.
3. Luo et al., (2008). Temporal moments for transport with mass transfer described by an arbitrary memory function in heterogeneous media. *WRR*, *44*(1).
4. Schmid, (2003). Temporal moments routing in streams and rivers with transient storage. *AWR*, *26*(9), 1021-1027.
5. McCallum et al., (2020). A Numerical Stream Transport Modeling Approach Including Multiple Conceptualizations of Hyporheic Exchange and Spatial Variability to Assess Contaminant Removal. *WRR*, *56*(3), e2019WR024987.

Further Information:

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