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Effect of temporal variability in infiltration on contaminant transport in the unsaturated zone

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Abstract

A general methodology has been developed for investigating the effect of short-term temporal variability in infiltration on the long-term transport of contaminants in soils. A one-dimensional, unsaturated transport model was used to simulate the transport of a sorbing, nonvolatile solute, using either steady-state or randomly varying infiltration. Concentration breakthrough curves are plotted against time and cumulative infiltration for constant rainfall, and for five, random-rainfall realizations. The observed time-based breakthrough curves for an individual year depend significantly on the actual rainfall pattern for that year. The average breakthrough curve, generated from many years of randomly generated rainfall, approaches the constant infiltration time breakthrough curve. For an individual year, the cumulative infiltration breakthrough curves for variable and constant infiltration match closely, as suggested by Wierenga, P.J. [Wierenga, P.J., 1977. Solute distribution profiles computed with steady-state and transient water movement models. Soil Sci. Soc. Am. J., 41, 1050]. This indicates that, for the conditions examined, cumulative rainfall can be used to predict adequately contaminant transport for a given time period. Under more severe conditions, increased variability in infiltration is expected to increase dispersion. A dimensional analysis of the governing equations indicates two additional explanations for the influence of infiltration variability on contaminant transport. First, the hydraulic conductivity (and therefore, the velocity) and retardation factor depend on the soil water content, which depends on the infiltration pattern. Second, molecular diffusion dominates transport during dry periods. The impact of this diffusion on the overall contaminant transport depends on the duration of dry periods.

Keywords: Unsaturated flow; Transport model; Hydrodynamic dispersion; Infiltration

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1. Introduction

Long-term (multi-year), unsaturated-zone models often predict solute transport based on average rainfall rates to represent infiltration. However, the temporal distribution of infiltration is important in determining the transport of solutes through the soil column. For example, dispersion may increase with increasing variability in infiltration. The goal of this work is to determine whether annual average rainfall rates can be used to accurately predict the accumulation of a sorbing, non-reacting, non-volatile solute in unsaturated soils over time scales of several decades.

Wierenga (1977) and Beese and Wierenga (1980) examined a related problem by modeling the transport of a spike of non-reacting solute through an irrigated agricultural soil. They modeled 100 days of infiltration, and compared constant infiltration to 2 h of irrigation every 10 days. They found that breakthrough curves for these two scenarios were similar, but that dispersion was two to three times greater when the infiltration was unsteady.

In contrast to these two studies, this investigation examines the effect of variable and constant infiltration and transport on the buildup of heavy metals in agricultural soils over several decades. To check the validity of our transport model, we used the inputs in Wierenga (1977) and Beese and Wierenga (1980), and compared the outputs. The same transport behavior was observed, indicating that any differences in our conclusions are only due to the different problem being studied.

2. Mathematical framework

The general advection–diffusion transport equation may be expressed in one-dimension as:

$$\frac{\partial(R\theta c)}{\partial t} = -\frac{\partial(u\theta c)}{\partial z} + \frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right), \tag{1}$$

where: t = time (s), c = concentration in the liquid phase (g/l), u = velocity (m/s), z = depth (m), θ = water content (m^3/m^3), D = effective diffusion coefficient (mm^2/s), and R = retardation coefficient, representing sorption of the solute onto the soil (unitless).

$$R = 1 + \frac{\rho K_d}{\theta} \tag{2}$$

where: K_d = partition coefficient (l/g); ρ = soil density (g/l).

In general, the solute transport equation (Eq. (1)) must be solved numerically. However, an approximate solution, which may be useful for understanding system behavior, may be found if some simplifying assumptions are made. An example of this approach is outlined in Appendix A and the consequent results are presented below.

3. Methodology

Solute transport through an unsaturated soil column is predicted here with a numerical model, using steady-state infiltration and varying infiltration rates. Comparison of model results indicates how temporal variability influences solute transport. A dimensional analysis, combined with perturbation analysis of the governing equations, was also conducted to provide a theoretical explanation for the effect of temporal variability in infiltration on solute transport.

4. Computational approach

A transient model of flow and solute transport through the unsaturated zone (Binning, 1994) was used in this investigation. The soil column is assumed to have no solute initially, and all infiltrating water has a relative solute concentration (c/c_0) of 1. The solute is non-volatile and non-reacting. The initial and boundary conditions and model parameters are listed in Table 1.

At each time-step, the infiltration through the top of the soil is given by the rainfall rate for that day. For the constant-infiltration case, the rainfall was held constant at the value of the annual average. To simulate variable infiltration, a daily rainfall rate was randomly generated as model input. At each time step, a random number was generated from a uniform distribution to determine whether it was raining during that time step (percent rain days). If it was raining, the rainfall rate was generated according to the log-normal distribution described in Smith and De Veaux (1992), with mean value of 750 mm/year, and coefficient of variation (CV) of 0.5 or 1.0.

The model was run for six cases, representing different combinations of percent rain days and CV of rainfall rate. Solute breakthrough curves were recorded at three depths (60, 200 and 380 mm). Fig. 1 shows concentration vs. time and vs. cumulative rainfall for the most variable rainfall scenario studied (rainfall rate has a CV = 1; rain occurs on 10% of the days).

Although the total annual infiltration is equal in all cases (750 ± 10 mm), the total rainfall at any point in time during the year may be different for each case, resulting in distinct breakthrough curves, even without the effects of dispersion (Fig. 1a). We are interested in investigating mechanisms other than pure advection for predicting transport. In order to accomplish this, we have used cumulative infiltration in our analysis, as described in Appendix A, effectively eliminating the dry periods between storms, to minimize the effects of variability in advective transport. The effect of variability in advective transport is clearly visible in Fig. 1a, but can also be observed in the cumulative infiltration plots (Fig. 1b), to a lesser extent. Because soil moisture, and hence, velocity, experiences greater fluctuations near the surface than at depth, and cumulative infiltration is measured at the surface, shallow depths exhibit larger deviations from the average breakthrough curve.

A comparison of the cumulative infiltration breakthrough curves illustrates the variations in total infiltration, at a given time, for different trials. Except for occasional

Table 1
Model parameters, initial conditions, and boundary conditions

Parameter	Symbol	Value	Units	Basis
Column height	H	680	mm	
Initial conditions				
Head distribution		Hydrostatic		
Contaminant concentration	C_0	0.0	mg/l	
Boundary conditions (bottom of column)				
Head	Ψ_H	-2500	mm	
Contaminant concentration	C_H	0.0	mg/l	
Rainfall				
Percent of rainy days		10–35%	% days	Van der Leeden et al., 1990
Mean annual rainfall		750	mm	Smith and De Veaux, 1994
Coefficient of variation (rainfall rate)	CV	0.5–1.0		Sturdevant et al., 1999
Soil and solute parameters				
	θ_r	0.035		Kool and Van Genuchten (1991), taken from a loamy sand
	θ_s	0.401		Kool and Van Genuchten (1991), taken from a loamy sand
Van Genuchten parameters				
	K_s	146.6		Kool and Van Genuchten (1991), taken from a loamy sand
	α_{vg}	0.115		Kool and Van Genuchten (1991), taken from a loamy sand
	n_{vg}	1.474		Kool and Van Genuchten (1991), taken from a loamy sand
Sorption coefficient	K_d	1.0	l/g	
Dispersivity coefficient	α	20	mm	
Soil bulk density	ρ_{bulk}	3.78	g/l	
Soil porosity	η	0.436		

lags, which have a duration of 1–2 days, the variable rainfall curves for cumulative infiltration fit very closely to the average rainfall case. When results are plotted in terms of cumulative infiltration, the effect of dispersivity is negligible. This is especially true when one considers typical uncertainties in the natural soil system.

A comparison of the plots for all six combinations of rainfall-rate CV and percent rain days (not shown) indicates that percent rain days, not CV, is the dominant factor in determining the shape of the breakthrough curves, and the difference from the constant infiltration case. Even with a large CV, as rain days approaches 100%, the time breakthrough curve approaches the constant infiltration case, because even with large variations in the daily rain rate, the cumulative rainfall oscillates closely around the

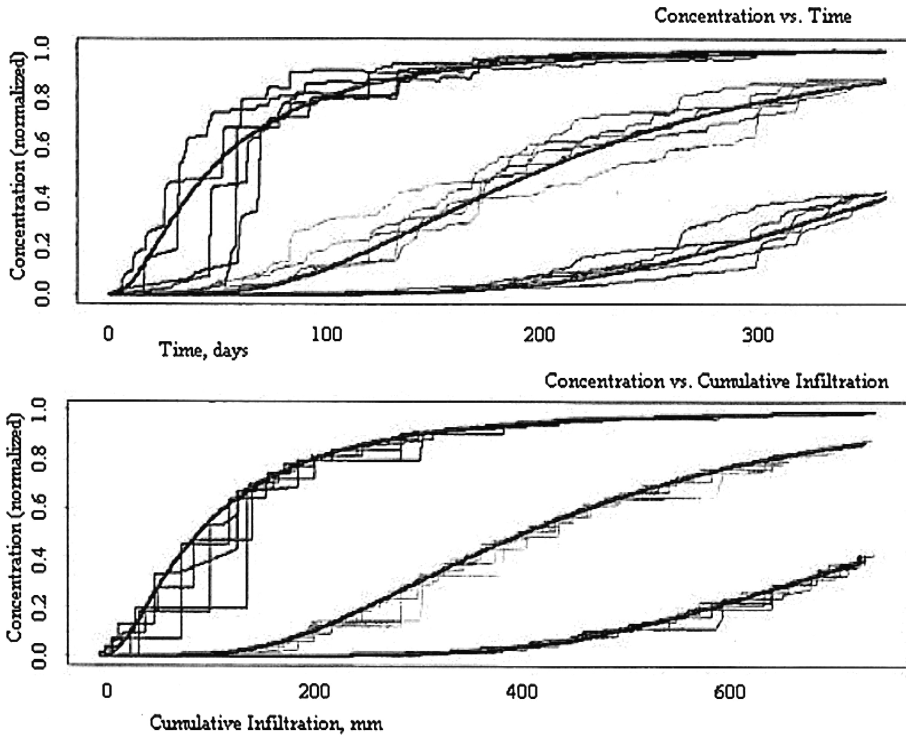

Fig. 1. Breakthrough curves for 10% rain days and CV = 1. Lines represent the six cases studied.

cumulative rainfall for the average infiltration case. Conversely, as percent rain days becomes small, even with CV = 0, the cumulative rainfall will have sudden jumps, and the time breakthrough curves will differ from the average infiltration case. With fewer rain days, the water velocity exhibits punctuate equilibrium: it is close to zero most of the time, and jumps up during the occasional storm. With more rain days, the water velocity at the surface exhibits spikes, the result of each storm, but the water deeper in the column (380 mm) flows more uniformly ($<$ 20 mm/day).

These results show that when variability in advection is corrected for, and only the influence of dispersion is observed, there appears to be no real difference between the variable-rainfall case and the constant-flux case, for the range of conditions in this study. The dispersivity coefficient does not need to be increased to incorporate an increase in the dispersion due to temporal variability in rainfall.

The effect of changing the dispersivity coefficient for the constant infiltration case is seen in Fig. 2. The plots shown represent a large range of dispersivities, from 0.1 to 200 mm, with the simulation for the value used for the constant infiltration case of Fig. 1a (20 mm) darkened. It is immediately obvious that the change in shape of the breakthrough curves is different for an increase in dispersion, compared to the change in

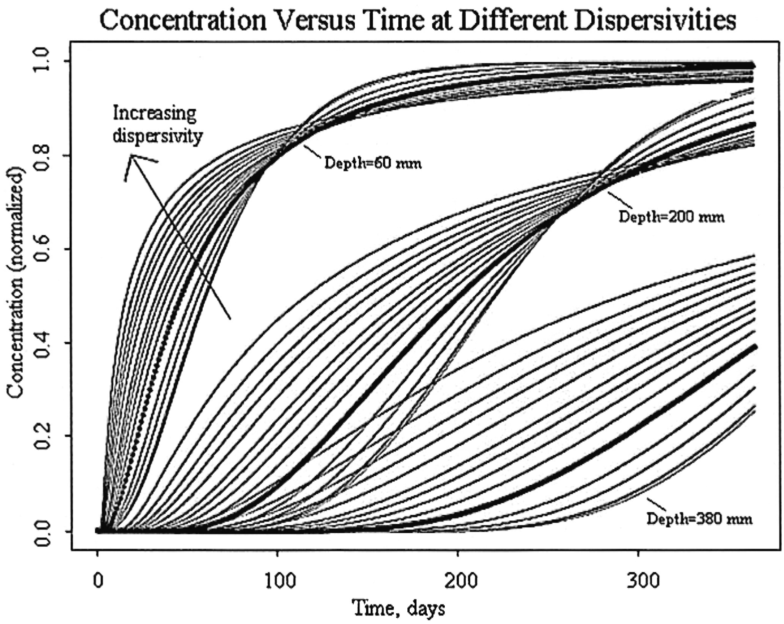

Fig. 2. Breakthrough curves with different dispersivity coefficients. Infiltration is constant in all cases, and the dispersivity coefficients range from 0.1 to 200 mm. The bold lines are simulations using a constant dispersivity coefficient of 20 mm at different depths.

shape from varying infiltration rates. Thus, it is not possible to simply modify the dispersivity coefficient to account for variability in the time breakthrough curves.

5. Dimensional analysis / perturbation analysis

To understand the variability observed in the time-based breakthrough curves, a dimensional analysis and perturbation analysis of the underlying equations was conducted. All of the variables (θ, u, R, c and D) are transient and spatially variable. In the general case, the transport Eq. (1) is solved numerically. However, insights into the governing processes can be gained by analyzing a simplified case. For example, in quasi-steady-state, the flow variables (u, θ) are approximately constant, while the concentration remains transient. If u and θ are assumed to be constant, $R(\theta)$ and $D(u)$ are also constant.

Because two mechanisms, advection and dispersion, affect transport, it is necessary to evaluate the effects of variable and constant flow on each of these mechanisms. As outlined in Appendix A, it is possible to calculate a ratio, r, which describes the relative importance of dispersion and advection. A second ratio, E, can be calculated as the ratio of r for a case of variable infiltration and constant infiltration. Using perturbation analysis (outlined in Appendix A), we can determine that the time average of E is not, in general, equal to 1. Thus, variations in velocity may influence the relative importance of dispersion and advection:

$$\bar{E} = \sqrt{1 + \frac{\overline{\langle \alpha\theta' u' \rangle}}{\bar{\theta}\left[\alpha\bar{u} + D_{\mathrm{m}} \right]}}\ , \tag{3}$$

where overbars indicate time-averaged quantities and primes indicate deviations away from the average value.

Temporal variability can influence transport in two ways. First, the history of water velocity variability will influence the history of water content and the relationship between the two. Thus, the time average of E will depend on the history of variations in velocity. A second influence of temporal variation may be observed if dispersion is a non-linear function of velocity. In this case, the time average of E will contain non-linear terms relating to the variations in the velocity. In the model considered for this work, dispersion is assumed to be linearly related to velocity, so this mechanism is not present, although some authors (de Marsily, 1986) have suggested a nonlinearity of dispersion with velocity.

One final insight can be taken from the equation for the time average of E. As the variations in θ or u (or both) become small, the effect of variability becomes smaller. By analogy to heat propagating into a semi-infinite medium with the surface temperature varying sinusoidally around a mean (Bird et al., 1966), there are two limiting cases under which the effect of these variations will be small. If changes in the rainfall rate vary rapidly around the mean, the variations will damp out quickly within the soil profile, and the velocity will be constant at most depths. If changes in the rainfall rate are slow, then each rainfall rate persists long enough for the velocity of the front to propagate deeply into the soil column. In both cases, the velocity at medium depths is at quasi-steady-state (changing slowly), and $\bar{E}$ approaches 1, which means there is no difference between constant infiltration and variable infiltration cases.

The conditions predicted by the ground water model indicate that the system is somewhere between these two cases, with a maximum $\bar{E}$ of 1.1. In general, velocities vary substantially around the mean, so that the first case, in which soil water velocities at most depths are approximately constant, is not observed. In a few cases, the second regime is observed: for a large rainfall event, the velocity profile reaches deep into the soil column. However, this is not usually the case, and it does not last more than a time step or two.

If we assume θ is constant, the advection–diffusion transport equation can be written in dimensionless form as (see Eq. A-4):

$$\frac{\partial c}{\partial \bar{t}} + \frac{\partial c}{\partial \bar{z}} = \left(1 + \frac{1}{R \cdot Pe(t)}\right)\frac{\partial^2 c}{\partial \overline{z^2}}\ , \tag{4}$$

where:

$$Pe(t) = \frac{\alpha\bar{u}U(t)}{D_{\mathrm{m}}} \tag{5}$$

is the time-dependent Peclet Number, representing the ratio of advection to diffusion. Diffusion now becomes important. If there is no molecular diffusion ($D_m \sim 0$; $Pe \gg 1$), the time dependence in the equation collapses, and the solution is identical for variable and constant infiltration. Only with molecular diffusion present does $Pe(t)$ change the solution to the equation.

This can be seen in the following two cases of infiltrating fronts, with constant θ. Molecular diffusion is the only mechanism for temporal variability to influence transport. In one case, the front moves slowly at a constant rate. In the second case, the front moves quickly to half way, is stationary for most of the time, and then quickly moves forward the second half at the end of the trial. In the first case, advection and diffusion occur simultaneously. In the second case, advection and diffusion dominate transport alternately. The contaminant breakthrough curves for these two cases will only be different due to molecular diffusion.

In many cases, diffusion is much smaller than dispersion. However, if there are long periods of no infiltration, such as what might occur in very arid regions, molecular diffusion would have time to act as a transport mechanism between rainfalls, leading to a different breakthrough curve for variable infiltration. This mechanism might affect the results of Beese and Wierenga (1980). In their study, infiltration was zero for 98% of the time (2 h of infiltration every 10 days). With a majority of the time spent in a diffusion-dominated regime, the influence of variability would be greater than was observed in the current study.

6. Summary

The effect of short-term temporal infiltration variability on the long-term transport of contaminants in soils was investigated. Daily rainfall was randomly generated for 1 year intervals, based on the percent of days receiving rain (10–35%) and the coefficient of variation in the rainfall rate (0.5–1.0); in all cases, the total rainfall was 750 ± 10 mm/year. Over the range of rain days and CVs of rainfall rates studied, percent rain days had a larger impact on the deviations from the mean transport (on days receiving rain) than the CV compared to the constant infiltration case.

Breakthrough curves for constant rainfall and for five realizations of variable rainfall were plotted against time and cumulative infiltration. The observed time-based breakthrough curves for an individual year depend significantly on the actual rainfall pattern for that year. The average time-based breakthrough curves over many years of randomly generated rainfall approach the constant infiltration time breakthrough curves.

Plotting concentration against cumulative infiltration transforms the time axis, and generates smooth breakthrough curves. For an individual year, the cumulative infiltration breakthrough curves for variable and constant infiltration match closely. This indicates that cumulative rainfall is adequate to predict contaminant transport for a given time period. Thus, use of constant infiltration rates rather than variable infiltration rates over many years will not result in significant error in estimating transport. This finding may result in significant savings in computational and data-collection efforts, as annual average data and longer time steps should be adequate for estimating transport of a conservative solute in soils for long-term simulations. The conclusions reached here differ from those of Beese and Wierenga (1980), whose work focused on an irrigation system with much larger infiltration variance, especially with respect to the amount of time the system was not receiving infiltration, and a shorter time frame. Under these specialized conditions, they found that dispersivity did need to be increased. This may be accounted for, in part, by the increased importance of molecular diffusion under the conditions they studied.

A dimensional analysis of the transport equation compares the relative importance of advection to dispersion, and gives a theoretical basis for the influence of variability in velocity on transport. A numerical solution is needed in the general case, when the variables are transient. However, the equations can be simplified under certain assumptions, to suggest explanations for the effect of infiltration variability on contaminant transport. Two such factors were identified in this study: transient water content and molecular diffusion. First, the hydraulic conductivity depends on the water content over time, which depends on the exact history of infiltration. Second, during dry periods, molecular diffusion becomes the dominant transport mechanism. The exact transport will depend on when and how long the soil experiences dry periods. In general, the effect of these factors is expected to be small in most naturally occurring systems.

Two additional factors that affect contaminant transport were identified, although they were not considered in this study. First, the water conductivity as a function of water content exhibits hysteresis. Thus, the conductivity depends on the exact history of rainfall. Second, if dispersion is a non-linear function of flow velocity, the exact history of infiltration will influence the mean dispersion, which will influence contaminant transport.

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Appendix A

A.1. Transforming time to cumulative infiltration

Dimensional analysis can suggest how time should be transformed to match the variable rate infiltration breakthrough curves with the constant infiltration curves.

The characteristic length scale is taken as the dispersion coefficient (α), and a characteristic velocity ($U(t)$) can be defined, to create dimensionless depth and velocity:

$$Z = \frac{z}{\alpha}; \quad V = \frac{1}{U(t)} \frac{u(t)}{R(t)}. \tag{A-1}$$

Substituting these into Eq. (1) yields:

$$\left(\frac{\alpha}{VU(t)}\right)\frac{\partial c}{\partial t}+\frac{\partial c}{\partial Z}=\left(1+\frac{D_{\mathrm{m}}}{\alpha R(t)VU(t)}\right)\frac{\partial^2 c}{\partial Z^2}. \tag{A-2}$$

Selecting as a characteristic time:

$$T=\int_0^t\frac{VU(\ddot{t})}{\alpha}=\int_0^t\frac{u(\ddot{t})}{\alpha R(\ddot{t})}\mathrm{d}\ddot{t}, \tag{A-3}$$

and recalling that $R(t)=R(\theta(t))$, the equation becomes:

$$\frac{\partial c}{\partial T}+\frac{\partial c}{\partial Z}=\left(1+\frac{D_{\mathrm{m}}}{\alpha VU(t)}\frac{1}{R(\theta(t))}\right)\frac{\partial^2 c}{\partial Z^2}. \tag{A-4}$$

By transforming time to T, any difference in the solution to the equation for variable infiltration compared to constant infiltration will arise from the term in front of the second derivative. This term incorporates the effect of variability in terms of θ and $u(t)$, as expected. The transformed time, T, is a constant times the cumulative infiltration. Thus, a plot of breakthrough curves vs. cumulative infiltration is expected to show the difference between the two cases that is due to temporal variability.

A second insight to be taken from this analysis is an understanding of how variability influences transport due to molecular diffusion. In the previous section, two mechanisms were shown for how variability could influence transport: $\theta(t)$ depends on the exact history of rainfall; and the dispersion coefficient might be a non-linear function of velocity (though it is not in this study). The non-linear effect does not hold for this study, but the dependence of θ on time does.

A.2. Analysis of effect of variable infiltration

The Peclet Number indicates the relative importance of advection and dispersion in terms of distance. With dispersion as a linear function of dispersivity ($D=\alpha u+D_{\mathrm{m}}$), the Peclet Number ($Pe$) is:

$$Pe=\left(\frac{L_{\mathrm{a}}}{L_{\mathrm{d}}}\right)^2=\frac{u^2 t}{R[\alpha u+D_{\mathrm{m}}]}=\frac{uL_{\mathrm{a}}}{R[\alpha u+D_{\mathrm{m}}]}. \tag{A-5}$$

The Peclet Number increases with time, indicating that the relative importance of dispersion decreases as the distance traveled increases.

To compare the effect of temporal variability on the Peclet Number, an enhanced transport ratio (E) can be defined as the ratio of Pe with variable velocity (u_{v}) to Pe with steady-state velocity (u_{c}). If $E=1$, the relative effect of dispersion is unchanged for variable velocity. On the other hand, if $E>1$, the relative effect of dispersion is more important for a variable velocity.

$$E=\frac{Pe_{\mathrm{c}}}{Pe_{\mathrm{v}}}=\left(\frac{L_{\mathrm{c}}}{L_{\mathrm{v}}}\right)^2\frac{R(\theta_{\mathrm{c}})[\alpha u_{\mathrm{v}}+D_{\mathrm{m}}]}{R(\theta_{\mathrm{v}})[\alpha u_{\mathrm{c}}+D_{\mathrm{m}}]}, \tag{A-6}$$

where subscripts v and c refer to conditions occurring with variable and constant infiltration, respectively.

One way to account for the variability in θ and u is:

$$\theta_{\mathrm{v}} = \bar{\theta} + \theta' u_{\mathrm{v}} = \bar{u} + u', \tag{A-7}$$

where overbars indicate time average values and primes indicate the variations (positive or negative) away from those averages. By definition, the time average of a variation is zero, and the constant velocity case is always at the average velocity and water content. The time average of the enhanced transport ratio becomes:

$$\bar{E} = \overline{\left\langle \frac{R(\theta_{\mathrm{c}})[\alpha u_{\mathrm{v}} + D_{\mathrm{m}}]}{R(\theta_{\mathrm{c}})[\alpha u_{\mathrm{c}} + D_{\mathrm{m}}]} \right\rangle} = 1 + \frac{\overline{\langle \alpha \theta'' u' \rangle}}{\bar{\theta}[\alpha \bar{u} + D_{\mathrm{m}}]}. \tag{A-8}$$

The time average term does not become zero because the flow velocity and the water content do not vary independently. Thus, $\bar{E}$ is not equal to 1, and variations in velocity can influence the relative importance of dispersion. For this study, $\bar{E}$ is calculated from the computational results as being approximately 1.05–1.1 on an annual basis. $\bar{E}$ may be larger on smaller time scales (a few storm events), although it will approach 1 on very small time scales (during part of one storm event).

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