

Effects of spatio-temporal variability of precipitation on contaminant migration in the vadose zone

Peng Wang,¹ Peter Quinlan,² and Daniel M. Tartakovsky¹

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[1] Annual meteorological data are routinely used in models of contaminant migration through the vadose zone. In arid and semi-arid regions, models based on such data yield negligibly small net infiltration rates that are insufficient to cause groundwater contamination. We conduct a series of flow and transport simulations, in which daily data from a weather station serve as input, to demonstrate that precipitation patterns typical of (semi-)arid regions make the reliance on annual data questionable. We demonstrate that the accuracy of temporally averaged predictions is influenced by the degree of nonlinearity of the Richards equation describing flow in partially saturated porous media. Additional errors are introduced when one ignores topographical and/or urban features that tend to focus and increase local infiltration rates. **Citation:** Wang, P., P. Quinlan, and D. M. Tartakovsky (2009), Effects of spatio-temporal variability of precipitation on contaminant migration in the vadose zone, *Geophys. Res. Lett.*, 36, L12404, doi:10.1029/2009GL038347.

1. Introduction

[2] The vadose zone forms a major hydrologic link, and acts as a main conduit for anthropogenic contaminants, between the Earth surface and groundwater aquifers. These two functions of the vadose zone are closely related, since the downward movement of water is the key mechanism of contaminant migration. Yet their respective analyses often require distinct methodologies and assumptions: even if large-scale averaged models are adequate to describe the effects of precipitation on groundwater recharge [e.g., *Izbicki et al.*, 2000, 2002], they might fail to ascertain the risk posed by contaminant spills to groundwater quality.

[3] This distinction becomes paramount in regions with arid or semi-arid climate, which is defined by annual rainfall below 250–500 mm (10–20 in). It is often argued that such low precipitation rates are not sufficient to drive contaminants from surface or near-surface spills to the water table, i.e., that contaminants released into soils in (semi-)arid regions pose no threat to groundwater quality.

[4] This assertion rests on an implicit assumption that time and/or space averaged precipitation rates provide an adequate input for subsurface flow and transport models. The highly nonlinear nature of both the coupling between surface and subsurface processes and the Richards equation

that is routinely used to describe flow in partially saturated porous media provides a clear indication that the superposition principle does not hold, i.e., that predictions based on averaged boundary conditions (infiltration rates) are at best an approximation. The adequacy of such approximations has been the subject of a handful of studies in the past few decades. Analyzing contaminant migration in homogeneous soils, *Wierenga* [1977] and *Beese and Wierenga* [1980] found breakthrough curves under time-varying and averaged boundary conditions to be similar, while *Bresler and Dagan* [1982] and *Russo et al.* [1989] concluded that contaminant might travel significantly faster and further under time-variable infiltration than under its time-averaged counterpart. *Destouni* [1991] attributed this discrepancy to the absence of root uptake from the latter studies and concluded that the use of time-averaged infiltration rates is justifiable. (Note that she considers infiltration rates typical of humid climates and calls for the use of modified soil parameters.) The more recent studies of *Marshall et al.* [2000] and *Schoups et al.* [2006] seem to support this finding, even though *Marshall et al.* [2000] cautioned that it might become invalid under severe weather conditions and *Schoups et al.* [2006] added a few caveats discussed below.

[5] Several crucial issues related to the adequacy of averaged precipitation rates as predictors of the risk of groundwater contamination remain unresolved. First, most of the studies mentioned above examined predictive errors stemming from the reliance on of average infiltration rates rather than their precipitation counterparts. While the latter are readily available on an hourly basis, e.g., from meteorological stations, the former have to be estimated. Second, the impact of the degree of nonlinearity of the Richards equation, i.e., of the choice of particular constitutive laws, has not been investigated. Finally, surface's topography and/or local land use localize infiltration, enhancing a contaminant's downward migration in a manner that undermines the utility of spatially averaged precipitation and infiltration rates. This letter aims to elucidate the impact of spatio-temporal averaging of precipitation rates on flow and transport predictions. This question gains in significance now that global climate change is likely to result in more severe weather with stronger rainfall, greater runoff, and longer periods of drought even if resulting annual precipitation rates might remain unchanged [*Lambert et al.*, 2008].

[6] Flow in the vadose zone, i.e., distributions of volumetric flux $\mathbf{q}(\mathbf{x}, t)$, pressure head $\psi(\mathbf{x}, t)$ and water content $\theta(\mathbf{x}, t)$ at any point $\mathbf{x} = (x_1, x_2, x_3)^T$ and time t , can be described by a combination of Darcy's law and the continuity equation,

$$\mathbf{q} = -K\nabla(\psi + x_3) \quad \text{and} \quad \frac{\partial \theta}{\partial t} = -\nabla \cdot \mathbf{q}, \quad (1)$$

¹Department of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla, California, USA.

²Dudek, Encinitas, California, USA.

respectively. A flow model is completed by specifying functional forms of unsaturated hydraulic conductivity $K = K(\theta)$ and retention curve $\psi = \psi(\theta)$. We assume that a porous medium is homogeneous (heterogeneity effects are discussed below). To be concrete, we set initial water content to its residual value, $\theta(\mathbf{x}, 0) = \theta_r$, and place the water table at $x_3 = -L = -150$ m. The boundary condition at the Earth surface $x_3 = 0$ is determined from atmospheric data and surface conditions. In the presence of ponding, $\psi = h_o$ where h_o denotes the height of standing water on a flat surface. In the simulations below, we set $h_o = 0$ m. In the absence of ponding, the boundary condition at $x_3 = 0$ is $q_3 = i$ if $P > 0$ and $q_3 = -e$ if $P = 0$. Infiltration rate i is computed from precipitation rate P , actual evaporation rate e , and runoff rate r over a unit area as $i = P - e - r$. A medium's initial saturation is expected to influence the impact of spatio-temporal averaging of meteorological data, here the soil is assumed to be dry. Finally, we employ a simple, linear relation between runoff and precipitation, $r = C_r P$ with $C_r = 0.1$, which is a reasonable approximation for (semi-)arid regions away from major rivers [Ackerman and Schiff, 2003]. More complex relations would add another nonlinear feedback into the system.

[7] Actual evaporation rate $e = \max\{e_p, e_v\}$, where e_p is potential evaporative demand of atmosphere and e_v is a soil's ability to conduct water to the surface. The latter can be defined as [Lapalla et al., 1987] $e_v = K r_s (\psi_a - \psi_s)$, where $\psi_s = \psi(x_3 = 0)$ is the pressure potential at the surface, and the pressure potential of atmosphere ψ_a is given by the Kelvin equation $\psi_a = RT/(M_w g) \ln H_r$, in which R is universal gas constant, T is absolute air temperature ($^{\circ}\text{K}$), M_w is molecular weight of water and g is gravity acceleration, and H_r is relative humidity. In the absence of surface crust and vegetation, surface resistance r_s equals the reciprocal of the distance from the top node to land surface; in our case, it is 10 m^{-1} .

[8] Potential evaporation rate e_p is calculated from measurements of net solar radiation R_n , vapor pressure p_v , air temperature T_c ($^{\circ}\text{C}$), and mean wind speed at two meters above the ground U_w by using a modified Penman equation [Pruitt and Doorenbos, 1977],

$$e_p = \frac{wR_n}{694.5(1 - 0.000946T_c)} + 24(1 - w)(p_s - p_v)f_w. \quad (2)$$

Here $p_s = 0.6108 \exp[17.27 T_c/(T_c + 237.3)]$ is saturation vapor pressure; $f_w = 0.030 + 0.0576 U_w$ is the wind function; and the weight function $w = \Delta/(\Delta + \gamma)$ where $\Delta = 4099 p_s/(T_c + 237.3)^2$, and psychrometer constant $\gamma = 0.000646 (1 + 0.000946 T_c) (101.3 - 0.0115 z + 5.44 \cdot 10^{-7} z^2)$ with z denoting the elevation of a weather station above the mean sea level.

[9] Migration of a conservative contaminant with concentration $c(\mathbf{x}, t)$ is described by advection-dispersion equation, $\partial c/\partial t + \nabla(\mathbf{u}c) = \nabla(\mathbf{D}\nabla c)$, where $\mathbf{u} = \mathbf{q}/\omega$ is the mean macroscopic velocity, ω is the porosity, and \mathbf{D} is the dispersion coefficient tensor. Initially, the soil is contamination-free, $c(\mathbf{x}, 0) = 0$, except for the layer $x_3 \in [-0.5 \text{ m}, -0.4 \text{ m}]$ where the concentration is $c_0 = 100 \text{ gm}^{-3}$.

[10] The raw meteorological data used in the simulations presented below come from a California Irrigation Management Information System (CIMIS) station located near Five

Points, Fresno County, CA at the surface elevation $z = 86.9$ m. The data set, freely available on line, contains measurements of daily precipitation, air temperature, solar radiation, relative humidity, wind speed and vapor pressure collected from 1983 to 2008. The average annual precipitation rate during this time period was 0.2 m/year , which is representative of semi-arid regions.

[11] Unless explicitly stated, the simulations reported below correspond to a sandy loam soil with porosity $\omega = 0.496$, residual water content $\theta_r = 0.15$, saturated hydraulic conductivity $K_s = 0.7 \text{ m/day}$, and van Genuchten constitutive relations

$$K_r = \left(1 - |\alpha\psi|^{\beta-1} D^{-\gamma}\right)^2 / D^{\gamma/2}, \quad D = 1 + |\alpha\psi|^{\beta}, \quad (3a)$$

$$\Theta = \left(1 + |\alpha\psi|^{\beta}\right)^{-\gamma}, \quad \Theta = (\theta - \theta_r)/(\omega - \theta_r), \quad (3b)$$

with parameters $\alpha = 0.847$, $\beta = 4.8$, $\gamma = 1 - 1/\beta$. In all transport simulations, we set molecular diffusion to $D_m = 10^{-6} \text{ m}^2/\text{day}$, longitudinal dispersivity to $\lambda_L = 0.1 \text{ m}$, and transverse dispersivity to $\lambda_T = 0.01 \text{ m}$.

[12] Numerical code VS2DT [Healy, 1990] is used for daily numerical simulations over 25 years. Evaporation is simulated in VS2DT by a two-stage process, which requires three inputs: potential evaporation e_p , pressure potential of the atmosphere ψ_a and the surface resistance r_s . Since VS2DT can treat the surface as either a precipitation or evaporation boundary, but not both at the same time, we divide each daily recharge period into two periods: first taking effective precipitation after runoff as infiltration, with rate modified so that total inflow mass remains the same; it is then followed by an evaporation period.

2. Effects of Temporal Averaging

[13] We start by analyzing the effects of temporal averaging of daily atmospheric data on the downward migration of moisture and contaminants. A one-dimensional soil column was discretized into 1500 cells, which puts the contamination source in the fifth cell from the surface. Figure 1c compares temporal evolution of the wetting front (defined as the leading edge of a moisture plume wherein water content exceeds its initial value) computed with the daily meteorological data described above and its counterparts resulted from monthly and yearly averages of these data. One can see that the yearly averages lead to predictions that are both quantitatively and qualitatively wrong, while monthly averages yield somewhat better predictions that still underestimate the extent of wetting. It is worthwhile recognizing that the use of daily data is in itself an approximation that averages instantaneous rainfall intensity albeit over shorter time intervals than monthly and yearly data do. Hence the actual errors introduced by the reliance on yearly meteorological data are even higher.

[14] The extent of subsurface contamination resulted from 25 years of infiltration is shown in Figure 1d. The annual (averaged) precipitation data predict a contaminant that remains practically immobile in its initial position, which is consistent with routine claims made for (semi-)arid regions. This prediction is, however, at variance with predictions obtained with daily and monthly meteorological data.

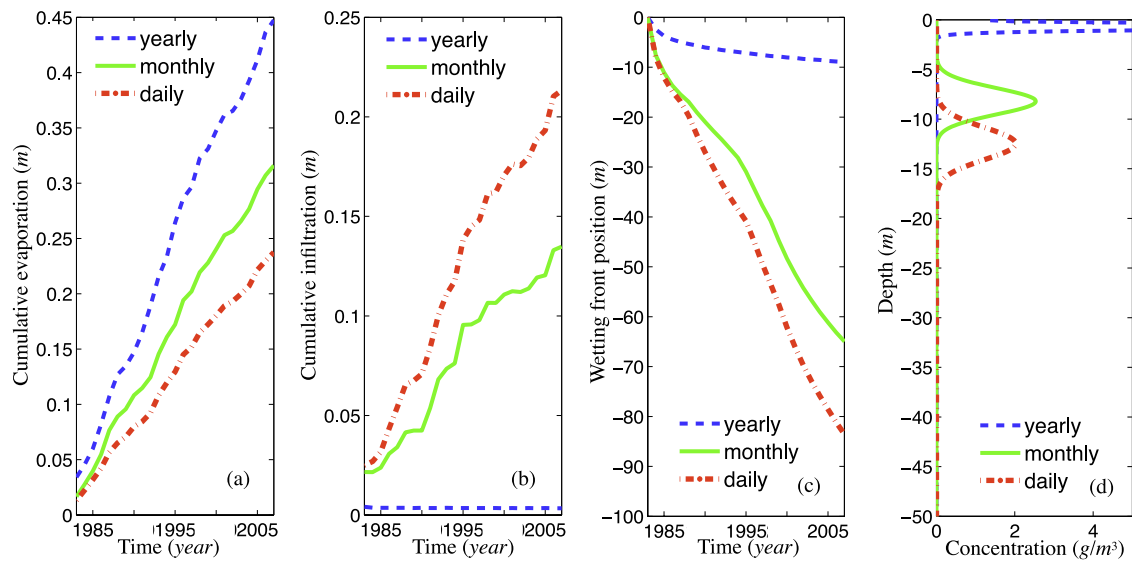


Figure 1. (a) Cumulative evaporation, (b) cumulative infiltration, (c) temporal evolution of the wetting front, and (d) final concentration profiles predicted with daily meteorological data and their monthly and yearly averages.

logical data. One can see that contaminant does migrate downward with reduced concentration, which reflects the presence of more water in soil in daily simulations than in their monthly and especially yearly counterparts.

[15] Figures 1a and 1b shed light on the cause of the apparent differences in modeling predictions based on daily, monthly, and yearly data. While yearly data result in zero infiltration, it is quite significant when computed from either monthly or daily data. Another important feature of these results is the increasing dichotomy between both infiltration and evaporation predicted from daily data and averaged data. At the end of 25 years, the actual evaporation computed from annual data is 0.447 m, which is almost twice the value of 0.2375 m computed from daily data. This finding is one of the reasons why *Destouni* [1991], whose simulations spanned a one-year period, observed little differences between predictions based on daily and annual data. Another reason is that we are concerned with (semi-) arid climates that are characterized by highly variable

precipitation patterns, while the simulations of *Destouni* [1991] were conducted for humid conditions.

[16] Both infiltration and contaminant migration in the vadose zone are influenced to a large degree by its hydraulic properties and heterogeneity. Figure 2 presents moisture profiles predicted with daily, monthly, and yearly averages for three homogeneous soil types: Fresno medium sand (saturated hydraulic conductivity $K_s = 400$ m/day), Columbia sandy loam ($K_s = 0.7$ m/day) and Yolo light clay ($K_s = 0.011$ m/day). Other hydraulic properties of these soils are given by *Lapalla et al.* [1987, Table 1]. The predictive errors caused by the reliance on annual meteorological data can be quantified in terms of a relative error introduced by the temporal averaging of meteorological data, $\mathcal{E} = |z_f^{(d)} - z_f^{(y)}|/z_f^{(d)}$ where $z_f^{(d)}$ and $z_f^{(y)}$ are the wetting front's positions resulting from the use of daily and yearly data, respectively. The errors increase with hydraulic conductivity, as wetting fronts travel farther and faster without reaching the water table ($\mathcal{E} = 90\%$ and 76% for Columbia sandy loam and Yolo

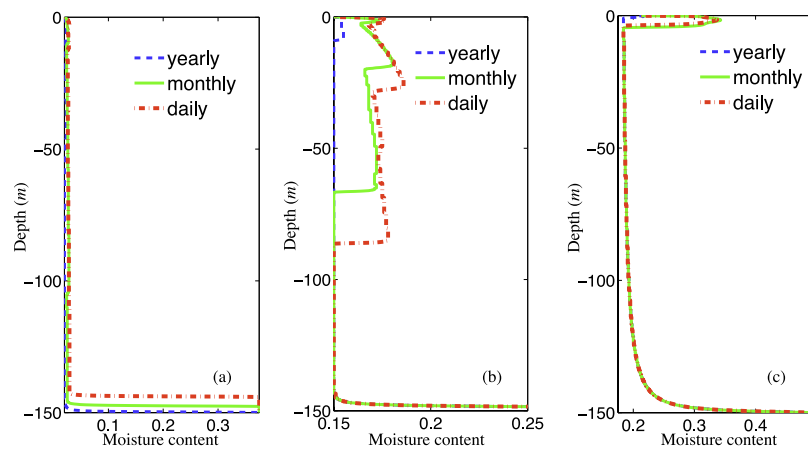


Figure 2. Moisture profiles at the end of 25 years of simulations for three soil types: (a) Fresno medium sand, $K_s = 400$ m/day; (b) Columbia sandy loam, $K_s = 0.7$ m/day; and (c) Yolo light clay, $K_s = 0.011$ m/day. These and other soil properties are taken from *Lapalla et al.* [1987, Table 1].

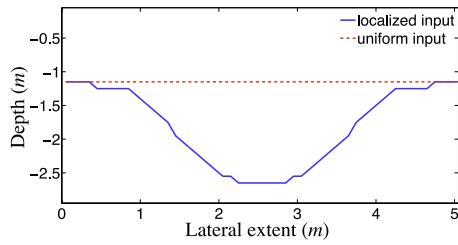


Figure 3. Extent of soil contamination after 25 years of simulations with spatially uniform and localized annual meteorological data.

light clay, respectively). After the wetting front reaches the water table, as is the case reported in Figure 2 for Fresno medium sand at the end of 25 years, this error decreases slightly to $\mathcal{E} = 68.5\%$.

[17] Detailed investigation of the impact of soil's heterogeneity lies outside the scope of this analysis. *Destouni* [1991] concluded that "Textural heterogeneity in the soil profile, such as a clay layer in sandy soft, increases the discrepancy between the steady state and the transient flow model when root water uptake is neglected." *Schoups et al.* [2006] seemingly contradict this conclusion by noting "Where time averaging does not give satisfactory results, it may still give adequate predictions of the spatial-ensemble distribution or statistical moments of the variable of interest." The veracity of such conclusions is hard to ascertain and is likely to be site specific.

3. Nonlinearity Effects

[18] Nonlinearity of the Richards equation (1) stems from the dependence of both relative hydraulic conductivity K_r and pressure head ψ on water content θ . The choice of constitutive relations $K_r(\theta)$ and $\psi(\theta)$ is bound to influence the discrepancy between predictions based on daily and yearly averages of meteorological data. To investigate this phenomenon, we compare predictions based on the van Genuchten model (3) with those corresponding to the Brooks-Corey model

$$K_r = (\psi/\psi_b)^{-2+3\lambda}, \quad \Theta = (\psi/\psi_b)^{-\lambda} \quad (4)$$

wherein $\psi_b = -0.85$, $\lambda = 1.6$ and $\theta_r = 0.11$, and the Haverkamp model

$$K_r = [1 + (\psi/\psi_a)^b]^{-1}, \quad \Theta = [1 + (\psi/\alpha)]^{-\beta} \quad (5)$$

wherein $\psi_a = -0.9$, $b = 9.2$, $\alpha = -1.26$, $\beta = 4.6$, and $\theta_r = 0.16$. The parameters in these models are representative of sandy loam soils [Lapalla et al., 1987, Table 1], except for ψ_a and b which were obtained by fitting. An alternative way to parameterize (4) and (5) is to ensure "hydraulic equivalency" between the three models (3), (4), and (5) [Morel-Seytoux et al., 1996; Tartakovsky et al., 2003]. The latter choice is more rigorous but less frequently used by practitioners.

[19] Our simulations revealed that the choice of a constitutive model affects both the wetting front penetration and cumulative infiltration. The Brooks-Corey model leads to

the largest \mathcal{E} , while the Haverkamp model results in the smallest error. After 25 years of infiltration, the relative error in wetting front predictions is $\mathcal{E} = 92\%$ for the Brooks-Corey model, 89% for Van Genuchten model and 79% for the Haverkamp model. We also found that the errors are largely insensitive to the value of saturated conductivity K_s .

4. Effects of Spatial Averaging

[20] Topographic features and built environments often focus infiltration. Under such conditions, the use of large-scale meteorological data to predict contaminant transport amounts to spatial averaging, which is bound to introduce predictive errors due to nonlinearity of the governing equation. We analyze this phenomenon by comparing contaminant migration induced by uniform and localized infiltration regimes. Both regimes use the same annual meteorological data as before; the former assumes uniform infiltration and evaporation over the land surface, while the latter focuses them at a point.

[21] Concentration isolines of $c = 0.01 \text{ g/m}^3$ at the end of 25 years of two-dimensional simulations with uniform and localized boundary conditions are shown in Figure 3. The spatial averaging of annual meteorological data underestimates the extent of downward contaminant migration from its initial location near the Earth surface ($x_3 = -0.4 \text{ m}$) by the factor of two. The increased water content resulted from localized infiltration results in a drop of solute volumetric concentration and a V-shaped concentration profile.

5. Conclusions

[22] In conclusion, (i) given high temporal variability of precipitation in (semi-)arid regions, the reliance on annual meteorological data might significantly underestimate the downward migration of contaminant; (ii) predictive errors stemming from the use of annual data increase with time and are more pronounced in highly conductive soils; (iii) selection of constitutive models for the Richards equation, e.g., van Genuchten model versus Brooks-Corey model, influences the magnitude of predictive errors; and (iv) surface topography and built environments further undermine the accuracy of predictions based on annual data by introducing errors associated with spatial averaging.

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- P. Quinlan, Dudek, 605 Third Street, Encinitas, CA 92024, USA.
D. M. Tartakovsky and P. Wang, Department of Mechanical and Aerospace Engineering, University of California, San Diego, 9500 Gilman Drive, Mail Code 0411, La Jolla, CA 92093–0411, USA. (dmt@ucsd.edu)