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Transfer Function Models of Solute Transport in Soil

*Sai Shree Pattnaik
Ph.D. Scholar, Department of Soil Science and Agricultural Chemistry, Odisha University of Agriculture and Technology, Bhubaneswar-751003
*Corresponding Author's email: saishreepatnaik2@gmail.com

Solute transport in soil controls the movement of dissolved nutrients, agrochemicals, and contaminants through the soil profile and is governed by processes such as advection, diffusion, dispersion, and soil and solute interactions. Mathematical models are widely used to describe and predict these processes. Among them, mechanistic models such as the Advection–Dispersion Equation (ADE) and dual-porosity or mobile and immobile models represent physical transport mechanisms in detail but often require extensive soil hydraulic and chemical parameters. In contrast, Transfer Function Models (TFMs) provide a simpler and efficient framework to relate solute input at the soil surface with its output at a given depth using travel-time distributions. TFMs capture the integrated effects of soil heterogeneity, preferential flow, and dispersion without explicitly simulating internal processes. Due to their computational efficiency and minimal data requirements, TFMs are widely applied for predicting nutrient leaching, pesticide mobility, and groundwater contamination risks, supporting improved irrigation, fertilizer management, and sustainable agricultural practices.

Introduction

Solute transport in soils refers to the movement of dissolved ions, nutrients, agrochemicals, and contaminants through the soil pore network driven by water flow processes such as infiltration, percolation, and groundwater movement. The behavior of solutes in soil is governed by advection, dispersion, diffusion, and chemical interactions (adsorption–desorption, precipitation–dissolution). Transfer function models provide a mathematical framework to describe the relationship between solute input at the soil surface and its subsequent breakthrough at a specified depth, without requiring detailed mechanistic soil-flow parameters. These models enable efficient prediction of solute leaching patterns in heterogeneous field soils, where traditional mechanistic models may be complex or data-intensive. Transfer function modeling plays a crucial role in evaluating nutrient leaching, pesticide mobility, and groundwater contamination risks.

Mechanisms of Solute Transport in Soil

The mechanisms governing solute movement are complex and highly non-linear, involving multiple interacting processes (Agah *et al.*,2017) such as :

A. **Advection/Convective movement**
B. **Diffusion/Molecular Diffusion**
C. **Dispersion / Hydrodynamic Dispersion**

- These processes are controlled by soil structure, texture, moisture regime, organic matter, and chemical gradients. Quantitative understanding of these mechanisms is achieved through mathematical models, which integrate these processes to simulate solute fate and transport dynamics under variable environmental conditions.

A. Advection /Convective Transport (Agah *et al*.,2017) :

- Advection, or convective transport, is the bulk movement of solutes carried by flowing water through soil pores. The flux of solute is proportional to their concentration (C):

$$q_c = q\,C$$

- The convective flux of solute passing through a unit area of soil expressed as

$$q_c = q\,C = -C(k)[\frac{\partial H}{\partial x}]$$

- To estimate distance of travel of solute per unit time, the mean apparent velocity or pore water velocity (v) is used: $v = \frac{q}{\theta}$
- Here θ is total volumetric water content of soil and solute flux (q_c) may also be characterized as: $q_c = v\theta C$.
- Advection dominates in saturated or rapidly draining soils, where the flow rate is high, such as during irrigation or rainfall infiltration.It is the primary mechanism responsible for leaching losses of mobile ions like nitrate (NO_3^-) and chloride (Cl^-) in agricultural soils.

B. Transport of Solutes by Diffusion (Agah *et al*.,2017) :

- Diffusion is the process by which a solute moves from region of higher concentration to region of lower concentration. This process is also known as molecular diffusion.
- It is assumed that the rate of transfer of solute by diffusion through a unit area of a section of soil is proportional to the concentration gradient.
- The diffusive flux is given by Fick's law: $q_d = -D_c \frac{\partial C}{\partial x}$
- Rate of diffusion (q_d) in bulk water, D_c is the molecular diffusion coefficient ($L^2\,T^{-1}$). In saturated soils, diffusion occurs within water-filled pores, whereas in unsaturated soils, tortuosity and discontinuity of water films reduce the effective diffusion coefficient ($D_e = \theta^m D_m$) here m accounts for tortuosity.
- Diffusion is significant in relatively stagnant zones, such as micropores or the immobile water phase of aggregated soils. The negative sign in equation is because diffusion occurs in the direction opposite to that of increasing concentration. The diffusion coefficient in porous media is lower than for bulk water as air and solid particles form barriers to liquid diffusion,
- The flux of diffusing solutes in an unsaturated porous medium is expressed in

$$q_d = -\theta D_s \frac{\partial C}{\partial x}$$

C. Hydrodynamic Dispersion Solute Transport (Agah *et al*.,2017):

- Differences in flow velocities at the pore scale (due to different pore sizes and shapes) cause the solute to be transported at different rates and thus leads to dispersion or mixing of an incoming solution within a pre-existing solution.
- This process is macroscopically similar to mixing by diffusion (thermal motion)
- It is passive (not driven by concentration gradients) and is entirely dependent on water flow. The solute flux due to mechanical (or) dispersion (q_h) is expressed by equation similar to Fick's Law for diffusion: $q_h = -\theta D_h \frac{\partial C}{\partial x}$. Where q_h is dispersive flux of solute, ($L\,T^{-1}$).
- D_h is the hydrodynamic dispersion coefficient ($L^2\,T^{-1}$) and C is concentration of solute in water (ML^{-3}). This coefficient is dependent on the interstitial pore water flow velocity (v [LT^{-1}]) and on the dispersivity (λ= [L]) of the soil which is a function of pore sizes and shapes according to: $D_h = D_h\lambda(\frac{q}{\theta})^n = \lambda v^n$. Where n is an empirical factor usually assumed to equal 1 (i.e., a linear dependency of D_h on v). The value of λ may range from 1 cm in small columns to a few meters in field experiments.
- In most cases the relative effect of hydrodynamic dispersion can exceed that of diffusion due to the macroscopic similarity between diffusion and hydrodynamic dispersion, it is

common to combine their coefficients (assuming that they are additive) into a diffusion-dispersion coefficient (D_e): $D_e(\theta, \mathrm{v}) = D_s + D_h$

- Where De is longitudinal hydrodynamic dispersion coefficient ($L^2\ T^{-1}$). De is referred to as the dispersion coefficient. It is also called the apparent diffusion coefficient or the diffusion- dispersion coefficient.

Model of Solute Transport in Soil

A. Mechanistic (physically based) models

- Mechanistic models use conservation laws and constitutive relations (physical laws which describes soil particles response to external force) to represent advection, dispersion, diffusion, sorption and reaction in porous media (Šimůnek *et al*., 2003).

1. **Advection–Dispersion Equation (ADE)**

- The Advection–Dispersion Equation is the most fundamental solute transport model which describes movement of solutes with mass flow movement of soil water (advection) and spread due to velocity variations and molecular diffusion (dispersion).
- It assumes the soil is homogeneous in nature, water flow is steady, and solute mixing follows Fick's law. ADE effectively represents uniform flow conditions but fails in structured or heterogeneous soils where solute movement is irregular, leading to early or delayed breakthrough. This process is expressed by equation:

$$\boxed{\frac{\partial(\theta C)}{\partial t} + \rho_b \frac{\partial S}{\partial t} = -\nabla \cdot (\theta \mathrm{v} C) + \nabla \cdot (\theta D \nabla C) + q}$$

(Šimůnek et al., 2003)

- $\nabla \cdot (\theta D \nabla C)$accounts for hydrodynamic dispersion combining mechanical and molecular diffusion. q represents source or sink processes such as fertilization, plant uptake, reactions, or leaching
- **Limitations.**
  - Fails to express flow through structured or highly heterogeneous soils. Dispersion coefficient is scale-dependent and often uncertain in field conditions

2. **ADE + Linear equilibrium sorption (Genuchten *et al*.,2013):**

- This model extends the basic Advection–Dispersion Equation by including solute interactions with soil particles through instantaneous, reversible sorption. It assumes a linear relationship between the solute adsorbed on the solid phase and that dissolved in the liquid phase.
- The model is useful for describing nutrient or contaminant retardation in soils but cannot represent nonlinear sorption, kinetic adsorption, or chemical transformations that often occur under real field conditions.

$$R\,\frac{\partial C}{\partial t} = -\mathrm{v} \cdot \nabla C + \nabla \cdot \left(\mathrm{D} \nabla C\right) - \lambda C + \frac{q}{\theta}, \quad R = 1 + \frac{\rho_b K_d}{\theta}. \qquad \textit{)Retardation)}$$

- R is the retardation factor accounting for solute–solid interactions, indicates how much slower a solute move through soil compared to water because some portion of those solute sticks (sorbs) to soil particles. $R = 1 + \frac{\rho_b K_d}{\theta}$,where $\rho_b$is soil bulk density.
- R=1 then no sorption, R>1 then there is sorption of solute on solid occurs . More is the value of R more is the sorption and more is retention of solute.
- $K_d$the distribution coefficient, and θ is volumetric water content. $\frac{\partial C}{\partial t}$ denotes the temporal change in solute concentration C.
- $-\mathrm{v} \cdot \nabla C$ represents advective transport with pore-water velocity v ; $\nabla \cdot (\mathrm{D} \nabla C)$ captures hydrodynamic dispersion. $-\lambda C$ accounts for first-order decay or transformation. q/θrepresents solute sources or sinks such as fertilization, plant uptake, or leaching.

3. **Dual-porosity / Mobile–Immobile (MIM) & Dual-permeability(Gerke & van Genuchten, 1993):**

- The dual-porosity or mobile–immobile model divides the soil water into two regions: a mobile zone where water and solutes move actively and an immobile zone where water is stagnant and solute exchange occurs only by diffusion. This approach captures non-equilibrium transport processes observed in aggregated or structured soils. It explains the slow release or tailing of solutes during leaching but oversimplifies real systems where pore connectivity and geometry vary continuously.

$$\theta_m \frac{\partial C_m}{\partial t} = -\frac{\partial(\theta_m v C_m)}{\partial x} + \frac{\partial}{\partial x}\left(\theta_m D_m \frac{\partial C_m}{\partial x}\right) - \alpha(C_m - C_{im}),$$

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = \alpha(C_m - C_{im})$$

$$\theta = \theta_m + \theta_{im}$$

- θ_m and θ_{im} represent the volumetric water contents of the mobile and immobile domains, respectively. C_m and C_{im} denote solute concentrations in each domain; v is the average pore-water velocity. D_m is the hydrodynamic dispersion coefficient in the mobile region.
- Explains rapid movement of surface-applied solutes (nitrates, pesticides) down macropores or tile drains in structured agricultural soils. Informs drain design and buffer strategies.

B. Transfer-Function Models (TFM) (Jury *et al*., 1986; Zhang, 2000).

- Transfer Function Models are empirical or semi-analytical tools that describe the relationship between solute input and output at a given soil depth without interrupting internal processes.
- TFMs are computationally simple and useful for large-scale agricultural applications or management decisions but lack physical realism and cannot directly represent mechanisms like sorption or preferential flow.

$$\boxed{\boldsymbol{C_{out}(t) = \int_{0}^{\infty} h\,(\tau)\, C_{in}(t-\tau)\, d\tau}} \qquad \textbf{)TFM)}$$

- where $h(\tau)$ is a probability density of travel times (first-passage kernel).Output concentration is superposition of past inputs delayed and spread by $h(\tau)$.
- **Agricultural relevance:** Operational forecasting of solute export (drainage concentrations, arrival timing) across many fields; supports landscape-scale risk screening and management scenarios.

Physical Interpretation of Transfer Function

- The transfer function can be interpreted as the residence time distribution (RTD) of solute particles within the soil profile.
- It reflects how long different solute fractions take to reach a given depth after infiltration.
- The shape and spread of $g(z,\tau)$ determine whether transport is uniform (narrow distribution) or highly dispersive (broad distribution).Various analytical forms of $g(z,\tau)$exist, each corresponding to a conceptual model of solute movement through the soil matrix.

Implementation of Solute Transport Models in Agriculture

- **Predict nutrient and contaminant movement:** Simulate the transport and fate of fertilizers, salts, and pesticides through the soil profile to understand solute dynamics under various field conditions.
- **Assess leaching and groundwater pollution risk:** Estimate potential nutrient or pesticide leaching beyond the root zone to protect groundwater and ensure environmental safety.

- **Optimize fertilizer and irrigation management:** Guide efficient use of fertilizers and water by identifying suitable. Application rates and timings that enhance nutrient uptake and minimize losses.
- **Understand soil–solute interactions:** Analyse key processes such as advection, dispersion, diffusion, and sorption that influence solute retention, mobility, and bioavailability in agricultural soils.
- **Support sustainable nutrient management:** Help design strategies for balanced nutrient cycling, reduced chemical inputs, and improved soil fertility over the long term.
- **Aid precision agriculture and environmental modelling:** Integrate with field data and digital tools to predict solute behaviour spatially, enabling site-specific management and environmentally sound decision-making.

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