International Journal of Web of Multidisciplinary Studies
(Peer-Reviewed, Open Access, Fully Refereed International Journal)
website: https://ijwos.com
Volume 3 Issue 2 , Feb 2026
OPEN ACCESS
E-ISSN : 3049-2424
DOI: https://doi.org/10.71366/ijwos

Estimation of Soil Solute Transport Parameters Using Small-Core Displacement Experiments Coupled with HYDRUS-1D Inverse Modeling: Technical description

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Article Info

Article History:

Published:28 Feb 2026

Publication Issue:
Volume 3, Issue 2
February-2026

Page Number:
474-479

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Abstract:

Accurate estimation of soil solute transport parameters is essential for predicting nutrient leaching and contaminant migration in agricultural and environmental systems. This study presents an integrated methodology combining laboratory displacement experiments on small soil cores with inverse modeling using HYDRUS-1D. Conservative tracer breakthrough curves were obtained under saturated steady-state flow conditions. Transport parameters were initially approximated using analytical solutions of the convection–dispersion equation and subsequently refined through inverse optimization. The inverse method simultaneously estimated longitudinal dispersivity and pore water velocity by minimizing discrepancies between observed and simulated concentrations. The results showed that inverse modeling significantly improved parameter accuracy and reduced uncertainty in comparison with analytical fitting. The proposed approach provides a robust and reliable framework for laboratory-based characterization of soil solute transport suitable for predictive modeling and environmental risk assessment.

Keywords: solute transport, breakthrough curve, dispersivity, inverse modeling, soil column experiment, HYDRUS-1D

1. Introduction

Understanding solute transport in soils is fundamental for evaluating the movement of nutrients, pesticides, and contaminants within the vadose zone[1] [2]. The increasing concern regarding groundwater pollution and sustainable agricultural practices has highlighted the need for reliable transport parameters[3] [4]. These parameters play a crucial role in predicting leaching processes and assessing environmental risks associated with intensive fertilization and irrigation [5] [6].

Solute movement in saturated and unsaturated porous media is governed by advection, dispersion, and diffusion processes [7]. Laboratory displacement experiments using soil columns have been widely employed to estimate transport parameters due to their simplicity and reproducibility [8]. However, classical analytical solutions of the convection–dispersion equation often rely on simplifying assumptions that may not adequately represent experimental conditions [9]. These limitations include neglecting transient hydraulic effects, boundary condition variability, and measurement uncertainties [10].

Inverse modeling has emerged as a powerful tool for parameter estimation by systematically adjusting model parameters to match observed data [11]. The numerical model HYDRUS-1D offers advanced capabilities for simulating water flow and solute transport under various conditions [12]. Its inverse module allows simultaneous optimization of hydraulic and transport parameters, providing improved accuracy compared to traditional analytical approaches [13].

The objective of this study was to develop and validate a combined experimental and numerical methodology for estimating soil solute transport parameters using small soil cores and inverse modeling. This approach aims to improve parameter reliability while reducing experimental time and cost.

2. Theoretical Background

Water flow in variably saturated soils is described by the Richards equation, which expresses the conservation of mass combined with Darcy's law [14]. The equation relates water content, pressure head, and hydraulic conductivity and allows simulation of transient flow conditions. Hydraulic properties are typically described using the van Genuchten–Mualem model, which has been widely adopted due to its flexibility and physical interpretation [15].

Solute transport in saturated porous media is commonly described by the one-dimensional convection–dispersion equation. This equation accounts for advection driven by water flow and spreading of the solute plume caused by mechanical dispersion and molecular diffusion [16]. The dispersion coefficient is expressed as the product of dispersivity and pore water velocity plus the molecular diffusion coefficient. Dispersivity represents the spatial variability of pore-scale velocities and is strongly dependent on scale and soil structure [17].

Inverse modeling involves minimizing an objective function representing the difference between observed and simulated concentrations. Numerical optimization methods such as the Levenberg–Marquardt algorithm are used to update parameters iteratively until convergence is achieved [18]. This approach allows simultaneous consideration of multiple processes and boundary conditions, improving the reliability of parameter estimation [19].

3. Materials and Methods

Undisturbed soil cores were collected from an agricultural field using stainless steel cylinders to preserve soil structure. The cores had a height of 20 cm and a diameter of 7.5 cm. After sampling, the cores were sealed and transported to the laboratory to prevent moisture loss and structural disturbance. Soil physical properties including bulk density, total porosity, and saturated hydraulic conductivity were measured using standard laboratory procedures.

The displacement experiment was conducted under saturated steady-state flow conditions. Soil cores were saturated from the bottom to remove entrapped air and ensure uniform water distribution. A constant hydraulic head was applied to establish steady flow. After achieving steady-state conditions, a step input of a conservative tracer solution based on potassium chloride was introduced at the column inlet. Effluent samples were collected at regular time intervals and analyzed using electrical conductivity measurements calibrated to tracer concentration.

Breakthrough curves were obtained by plotting relative concentration against time. Initial estimates of pore water velocity and dispersion coefficient were obtained by fitting analytical solutions of the convection–dispersion equation to the experimental data. These initial values served as starting points for the inverse modeling procedure.

The HYDRUS-1D model was used to simulate the displacement experiment. The model domain corresponded to the soil column length and was discretized using a uniform finite element mesh. The upper boundary condition was defined as a constant flux corresponding to the experimental flow rate, while the lower boundary was set as free drainage. The initial solute concentration in the column was set to zero.

The inverse modeling procedure involved fitting simulated breakthrough curves to experimental observations. The parameters selected for optimization included longitudinal dispersivity and pore water velocity. In some cases, saturated hydraulic conductivity was also refined to improve model performance. Optimization was performed using the built-in nonlinear regression algorithm [20].

Model performance was evaluated using statistical indicators including the coefficient of determination, root mean square error, and Nash–Sutcliffe efficiency [21]. These criteria were used to assess the agreement between observed and simulated concentrations.

4. Results

The experimental breakthrough curves exhibited a relatively symmetrical shape with limited tailing, indicating homogeneous transport conditions and absence of significant preferential flow [22]. The initial arrival of the tracer occurred close to the theoretical residence time, suggesting good control of hydraulic conditions during the experiment [23] [24].

Analytical fitting provided reasonable estimates of transport parameters; however, discrepancies were observed near the peak and late-time tail of the breakthrough curves. Inverse modeling significantly improved the fit between simulated and observed concentrations [25] [26]. The optimized parameters showed slight reductions in both pore water velocity and dispersivity compared to analytical estimates. This adjustment resulted in improved representation of the tracer front and peak concentration [27] [28].

The statistical indicators confirmed the superiority of the inverse approach. The coefficient of determination exceeded 0.98, and the Nash–Sutcliffe efficiency was greater than 0.95, indicating excellent agreement between simulations and observations. The root mean square error was significantly reduced after inverse optimization.

5. Discussion

The results demonstrate the effectiveness of combining displacement experiments with inverse modeling for estimating soil transport parameters [29]. The inverse approach allowed incorporation of realistic boundary conditions and reduced errors associated with analytical assumptions [30]. The method also accounted for measurement uncertainties and minor deviations from ideal experimental conditions [31].

The dispersivity values obtained were consistent with those reported in the literature for similar soil textures and laboratory scales [32]. The observed scale dependence of dispersivity confirms the importance of considering spatial variability when extrapolating laboratory results to field conditions [33].

The reliability of the method depends on the quality of experimental data and appropriate selection of optimized parameters [34]. Excessive parameterization may lead to non-uniqueness and instability in inverse solutions. Therefore, careful experimental design and sensitivity analysis are recommended [35].

6. Conclusion

This study presented a combined experimental and numerical approach for estimating soil solute transport parameters using small soil core displacement experiments and inverse modeling. The inverse procedure significantly improved parameter accuracy compared with analytical fitting. The methodology is efficient, reproducible, and suitable for laboratory characterization of soil transport properties. The approach is recommended for environmental and agricultural applications requiring reliable prediction of solute movement.

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