



Evaluation of CDE and MIM Models to Simulate TCE Transport in a Carbonate Porous Media

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ABSTRACT: It is essential to simulate the transport of this pollutant, especially in the industrial areas. In this research, an inverse solution has been employed to simulate the movement of TCE (Trichloroethylene). To evaluate the inverse solution, HYDRUS-1D and STANMOD software were used with two transport models including: Convection-Dispersion (CDE) and Mobile-Immobile (MIM). set of data from Yolcubal and Akyol (2001) were used at three TCE concentrations of 110, 113 and 1300 mg/L. The research was conducted on the loamy-sand and carbonate soil with a mean bulk density of 1.2 g/cm³. Experiments were carried out in columns with a length of 15 cm. At different time step, the water samples of the column output were taken to determine the TCE concentration and the breakthrough curves (BTC). The results of HYDRUS and STANMOD showed that the MIM model had a higher correlation coefficient than the CDE model with respect to the match BTC. The minimum error was zero for estimation of the dispersion coefficient at CDE where it is 3.5% at MIM. The error rate was minimum at the concentration 113 mg/L for adsorption isotherm coefficients in the inverse numerical solution and the same result for retardation factor in an inverse-analytical solution.

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1. INTRODUCTION

Trichloroethylene (TCE) is one of the main products of the petrochemical industry. TCE is used in the removal of grease from the surface of metals, household, and commercial solvents, paint cleaners, disinfectants, firefighters, and anesthetic substances. It is also used in various industries including automotive, metals, dyeing, electronics, steel, and wood.

It is essential to simulate the transport of this pollutant, especially in industrial areas. The allowed concentration of TCE is 5 µg/L for MCL based on EPA standard [1].

Numerical methods for soil pollution transmission were first used for soil-water modeling in the early 1960s, and a wide range of them was developed using the finite difference method in the last 20 years. Today, numerical models in the form of various computer programs are used by researchers for a wide range of initial and boundary conditions of water and salt transport in soil and conditions such as plant response to water regimes, nitrogen deposition, and deformation, irrigation water management, salts, and wastewater. Although these models are more flexible than analytical models so that they are more effective in stimulating the transfer of salts in the field, the definite nature of these models makes them difficult to use because of the spatial variability of the soil hydraulic properties. These models are extensively used for

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research work. Among the numerical and one-dimensional models of water and solute transport in soils under saturated and unsaturated environments, it can be mentioned to HYDRUS-1D, SWAP, WAVE, and MACRO models and for analytical models to STANMOD. Application of models can significantly save time and money, but this prediction is useful when it will consider the accuracy and validity of the model in these estimations. Therefore, the efficiency of the pollution transmission models for the solute should be evaluated.

The Hydrus-1D model is one of the advanced models associated with the one-dimensional movement of water and solute in the soil. This model which includes the numerical solution of equations) Convection-Dispersion Equation, CDE). The equations can simulate the movement of pollution in saturated and unsaturated conditions. This model estimates the soil properties by the inverse method [2].

The STANMOD computer software is developed for evaluating solute transport using analytical solutions. The CXTFIT 2.0 may be used to estimate parameters for transport during steady one-dimensional flow by fitting the parameters to the observed laboratory. The inverse problem is solved by minimizing an objective function that consists of the sum of the squared differences between observed and fitted concentrations.

The main objective of this research is an inverse solution



that has been employed to simulate the movement of TCE. To evaluate the inverse solution, HYDRUS-1D as a numerical solution and STANMOD as an analytical solution software was used with two transport models; DE and MIM (Mobile-Immobile model).

2. METHODOLOGY

In this study, a set of data from Yolcubal and Akyol (2011) were used. They injected TCE into soil columns (carbonate soil) at three concentrations of 110, 113, and 1300 mgL⁻¹[3]. In a caliche soil, the TCE absorption rate is 100 times less than in organic soils. The predominant calcium carbonate portion in the soil causes high TCE absorption. The rate of non-absorption of TCE in carbonate soils is high due to the presence of calcium carbonate, and then this rate decreases, while the organic matter in organic soils causes TCE to be absorbed. The caliche soil has a poorly sorted sandy loam texture with a mean grain diameter of 0.12 mm. The specific surface area of the soil is 0.383 m²g⁻¹. Caliche soil is composed of predominantly calcium carbonate (96%), minor amounts of quartz (2.12%), and organic carbon (0.97%). The column which has been used in the experiments was made of borosilicate and has a dimension of 4.8 cm and 15 cm in length. Column experiments were conducted at the different flow rates (Q=0.5 and 1 mL.min⁻¹) and the initial TCE concentrations (Co=110 and 1300 mg L⁻¹) under the saturated flow conditions. The columns were repacked for each test with the dry soil and then it was saturated with the deionized water. Before TCE column experiments, conservative tracer tests were conducted with PFBA (300 mg.L⁻¹) or Bromide (200 mg.L⁻¹) tracers to determine hydrodynamic flow conditions in the porous media. Following the completion of the tracer test, reactive tracer (TCE) was introduced to the same column continuously until the effluent concentration reached the influent concentration (C=Co). Then the TCE was eluted from the column by water flushing. During the experiment, effluent samples with high TCE concentrations (>1 mg.L⁻¹) were collected at the column outlet using a gas-tight Luer lock syringe, and TCE concentrations were measured immediately after sampling.

Samples belonging to low TCE concentrations (<1 mg.L⁻¹) were kept in a refrigerator in the vials having no headspace until analyzed for TCE. The column experiments continued until the effluent TCE concentration dropped below the detection limit or reached the stable concentration. TCE and non-reactive tracer breakthrough curves were obtained by plotting relative concentration (C/Co) versus pore volume (PV). High TCE concentrations (>1 mg.L⁻¹) in the samples were determined using a Varian Carry 50 UV-VIS spectrophotometer at a wavelength of 200 nm. The low TCE concentrations (<1 mg.L⁻¹) in the samples were measured by gas chromatography with Electron Capture Detector.

The general form of the sorption isotherm is represented by the following equation:

$$S = \frac{K_d C^m}{1 + \eta C^m} \tag{1}$$

Where S is the solute concentration in the adsorbed phase (M M⁻¹); C is the solute concentration in the aqueous phase; K_d is the oil-water partitioning coefficient; η is dimensionless-linearity exponent describing the heterogeneity of sorption sites having different affinities for retention. If η is unity, Eq. (1) would be linear.

In this research, the inverse numerical solution of TCE transmission with HYDRUS-1D software and the analytical inverse solution was performed with STANMOD software with two CDE and MIM models. An inverse solution method is one of the indirect methods for estimating effective parameters and it is an optimization method that can estimate the parameters by minimizing a target function, and this method is used more in saturated conditions [2]. In initial conditions, analysis of soil samples before the beginning of the experiment showed that the concentration of TCE in all soils was negligible. C(x,0)=0. For input boundary conditions, the concentration and duration of TCE injection are as well as the concentration of observation at different times of the TCE (breach curve). The breakthrough curve in STANMOD software was the volume of pore volume (PV) from the concentration to initial concentration (C/C0 ratio).

Outputs yielded by software implementation with two CDE and MIM models include estimated latency factor coefficients, diffusion coefficient, and absorption isotherm and penetration curve. To compare and evaluate the efficiency of the models, two square error-corrected parameters (RMSE) and correlation coefficient r were used which their values were calculated from Eqs. (2) and (3).

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (y_{pi} - O_i)^2}{N}} \tag{2}$$

$$r = \frac{N \sum_{i=1}^N O_i y_{pi} - \sum_{i=1}^N O_i \sum_{i=1}^N y_{pi}}{\sqrt{N \sum_{i=1}^N O_i^2 - \sum_{i=1}^N O_i^2 \times (N \sum_{i=1}^N y_{pi}^2 - (\sum_{i=1}^N y_{pi})^2)}} \tag{3}$$

3. RESULTS AND DISCUSSION

The results of the Hydrus model showed that the highest error rate was in the estimation of coefficient sorption isotherm (k_d) and the lowest percentage error was observed in the estimation of the dispersion coefficient (Table 1).

In all concentrations, the percentage error of the retardation factor was significant, which may be due to the lack of input of soil's properties such as bulk density and soil moisture content in STANMOD software. The estimated error of the retardation factor is more than HYDRUS (Table 2).

The breakthrough curve was fitted with estimated inverse data with STANMOD software by MIM and CDE models at 110, 113, and 1300 mg L⁻¹ concentrations. It showed that the CDE model had the highest error in the concentration of 110 and 1300 mg L⁻¹. The MIM model had a lower error and a better correlation coefficient than the CDE model in fitting the breakthrough curve at the concentration of 113 mg L⁻¹ (Fig. 1).

The breakthrough curve was fitted with estimated inverse

Table 1. Estimated error value of the inverse solution of HYDRUS software with CDE and MIM model

TCE concentration(mg/l)	Model	D	R	m	K _d
110	CDE	0	11	19	26
	MIM	48	26	13	26
113	CDE	14	9	3	128
	MIM	0	8	53	128
1300	CDE	31	7	3	9
	MIM	31	8	10	2

Table 2. Estimated error value of the inverse solution of STANMOD software with CDE and MIM model

R	D	Model	TCE concentration(mg/l)
48	3.5	MIM	110
11	21	CDE	
128	3.5	MIM	113
185	21	CDE	
45	3.5	MIM	1300
9.1	37.9	CDE	

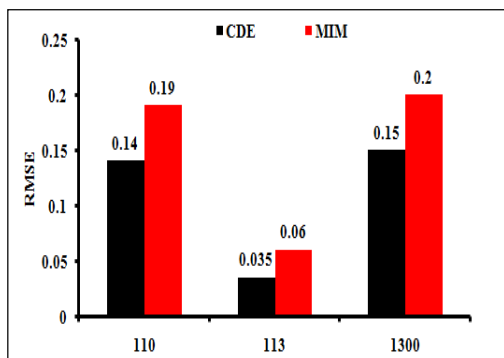


Fig. 1. Correlation coefficient simulation of inverse solution of STANMOD software with CDE and MIM model

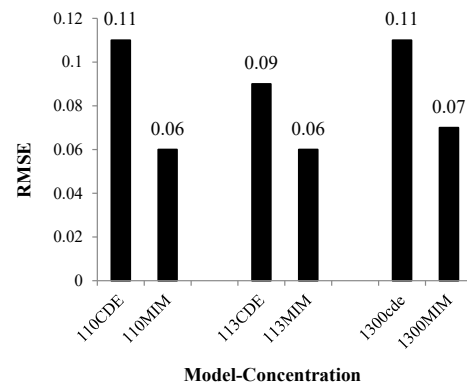


Fig. 2. Correlation coefficient simulation of inverse solution of HYDRUS software with CDE and MIM model.

data with STANMOD software and MIM and CDE models at 110, 113, and 1300 mg L⁻¹ concentrations which showed that the MIM model had a lower error in simulation breakthrough curve compared to the CDE model (Fig. 2).

4. CONCLUSIONS

Comparison of correlation coefficients and error in two software showed that inverse numerical solution was better than an analytical solution at concentrations of 113 and 110 mg L⁻¹. The estimation of coefficients in HYDRUS-1D has fewer errors in comparison to the STANMOD because HYDRUS-1D needs inputs of soil hydraulic characteristics as well as the parameter of pollution equations and if these characteristics such as soil saturated moisture and hydraulic conductivity (in this research these items were not measured) measure accurately, it will have a significant effect on the accuracy of the models in estimating the coefficients and even the fitting of the penetration curve. Models are sensitive to input values

so it will affect the simulation results, and the more inputs of the model with more reliable limits, the lower the error of the model. The lowest error rate in the estimation of the emission factor was zero and 3.5% in the second-order CDE and non-equilibrium, respectively. The highest estimation errors in STANMOD and HYDRUS-1D software were related to the retardation factor and adsorption isotherm coefficients at a concentration of 113 mg L⁻¹ in the MIM model, respectively.

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