Verification of T2VOC Using an Analytical Solution

for VOC Transport in Vadose Zone

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T2VOC represents an adaption of the STMVOC [*Falta and Pruess*, 1991] to the TOUGH2 [*Pruess*, 1991] environment. In many contaminated sites, transport of volatile organic chemicals (VOC) is a serious problem which can be simulated by T2VOC. To demonstrate the accuracy and robustness of the code, we chose a practical problem of VOC transport as the test case, conducted T2VOC simulations, and compared the results of T2VOC with those of an analytical solution. The agreements between T2VOC and the analytical solutions are excellent. In addition, the numerical results of T2VOC are less sensitive to grid size and time step to a certain extent.

Problem of the Test Case

The problem of the test case is a one-dimensional vertical transport of VOC in a homogeneous vadose zone caused by an instant release of VOC in the soil. In this study, the ground-water table is assumed at a depth of $d_3=30m$, and at the depth interval of $d_1=9m$ to $d_2=10m$ there is trichloroethylene (TCE) contamination with an initial uniform total concentration of $C_0=100\mu g/cm^3$ (Figure 1). We have chosen a small value for the initial total concentration such that the non-aqueous phase liquid (NAPL) does not exist and such that the density-driven gas-phase advection is insignificant.

Some major transport mechanisms considered in the simulations are (a) the advection of dissolved TCE through the aqueous phase with a constant infiltration rate, (b) the diffusion of TCE vapor through the gas phase, and (c) the adsorption of dissolved TCE to the soil matrix. The soil properties used in the simulations are the saturated hydraulic conductivity of $K_s=0.001cm/s$, a porosity of $\phi=0.5$, the *van Genuchten* parameters $\alpha=0.05cm^{-1}$ and $n=2$, a residual volumetric moisture content of $\theta_r=0.05$, and the fraction organic carbon $f_{oc}=0.001$. The dry bulk density of the soil is $\rho_b=1.325g/cm^3$ which is calculated by using the porosity and a typical value of $2.65g/cm^3$ for the mass density. At the land surface, a constant infiltration with a Darcy velocity of $v_L=1cm/yr$ is assumed through the simulation time. Since an instant equilibrium between phases is assumed by both the analytical solution and the numerical code, we only need to examine the concentration profile in either phase, e.g., the aqueous phase in this study.
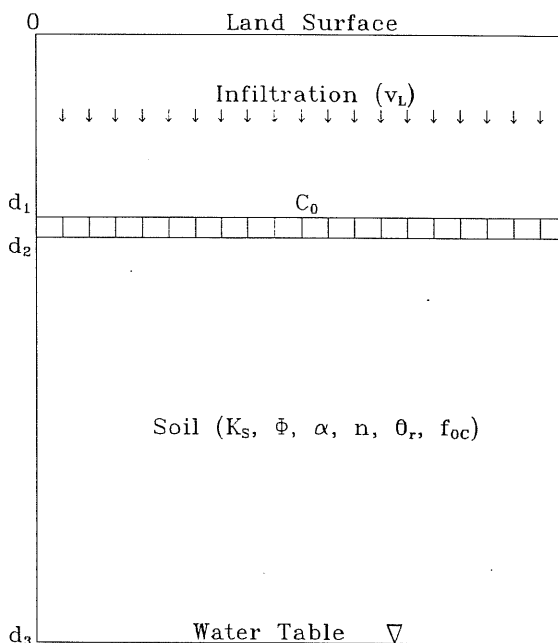

Fig. 1 Schematic view of the problem

The Steady-State Moisture Profile

Since we need to assume a steady-state moisture profile for the analytical solution [*Shan and Stephens*, 1994], it is necessary to generate such a moisture profile using either T2VOC or a simple analytical solution. The analytical solution for the one-dimensional vertical steady infiltration is simply the integration of the Darcy's equation

$$v_L = K\left(1 - \frac{d\psi}{dz}\right) \qquad (1)$$

where z is the vertical coordinates with the origin at the land surface, positive downwards; and K is the unsaturated hydraulic conductivity that is a function of the pressure head ψ via the *van Genuchten* [1980] model. Integrating the equation from the water table to an arbitrary depth, z, we obtain

$$z = d_3 + \int_0^\psi \left(1 - v_L/K\right)^{-1} d\psi \qquad (2)$$

which can be calculated by numerical integration. The calculated pressure head profile can be converted to a

moisture profile by further application of the *van Genuchten* model. The calculated steady-state moisture profile is represented by the solid line in Figure 2. We then used the same parameters and boundary conditions for two T2VOC flow simulations, one used a uniform grid size of $\Delta z = 1m$ and the other used a uniform grid size of $\Delta z = 0.1m$. The results are compared with the analytical solution in Figure 2. The agreements are excellent.
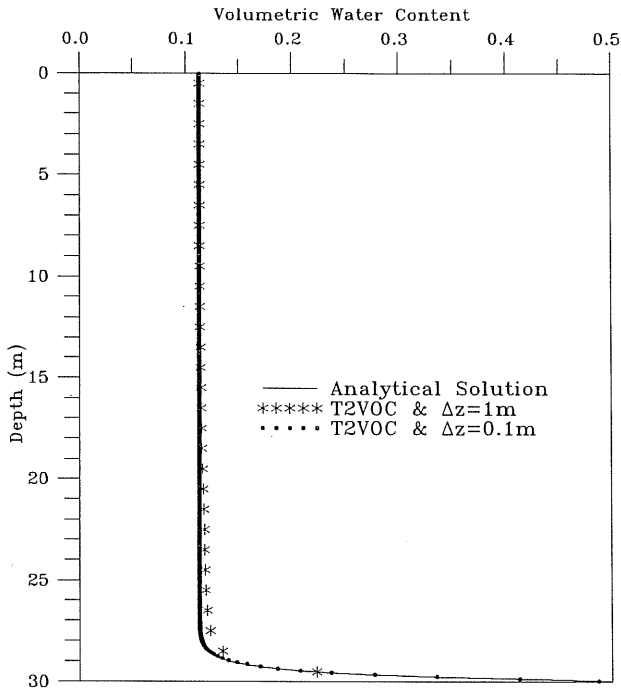

Fig. 2 Comparison of calculated steady-state moisture profiles

TCE Concentration in Water

The constant moisture content ($\theta = 0.112$) on the upper part of the curve in Figure 2 is used for the concentration calculation using the analytical solution [*Shan and Stephens*, 1994]. In applying the analytical solution, we have neglected the gas phase advection and adsorption, the dispersion in both the aqueous and the gas phases, and the biodegradation. The TCE properties used for analytical solution are exactly the same as those used in T2VOC, e.g., the partition coefficient $K_{OC} = 0.1 m^3/kg$ (input data to T2VOC), the gas diffusion coefficient $D_g = 7534 cm^2/d$ (calculated using T2VOC model), and the dimensionless Henry's constant $K_H = 0.2765$ (calculated from T2VOC). A constant temperature of 15°C was used for the T2VOC simulation.

The moisture profiles calculated by T2VOC using two different grid sizes were used as the initial conditions of flow for corresponding VOC transport simulations. For each grid size simulation, two runs
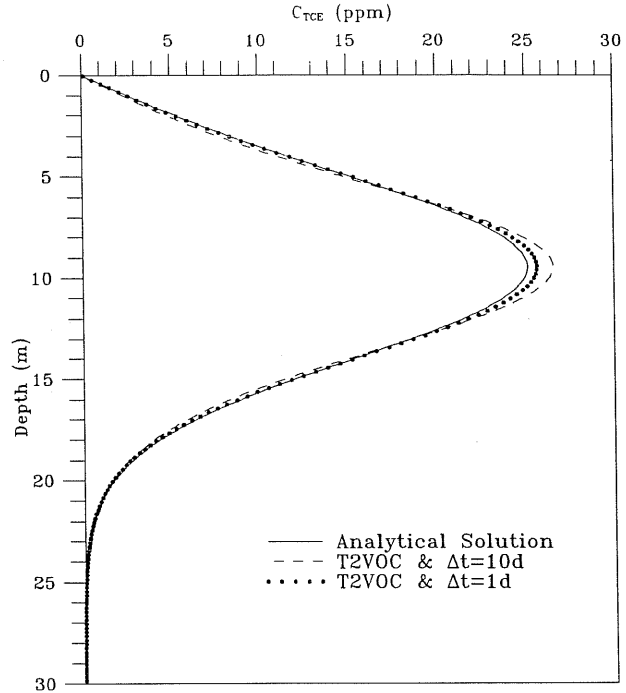

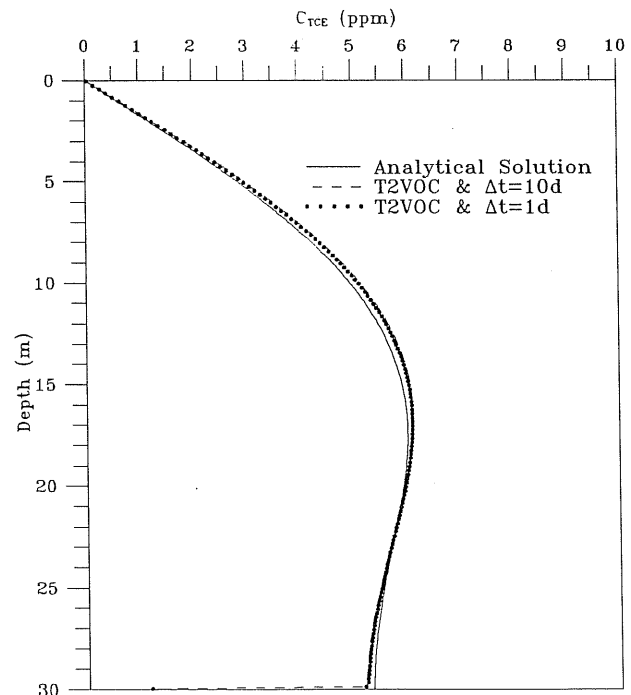Fig. 3a Comparison of calculated TCE concentrations in the aqueous phase at $t = 100d$ (constant $\Delta z = 0.1m$)

Fig. 3b Comparison of calculated TCE concentrations in the aqueous phase at $t = 1000d$ (constant $\Delta z = 0.1m$)
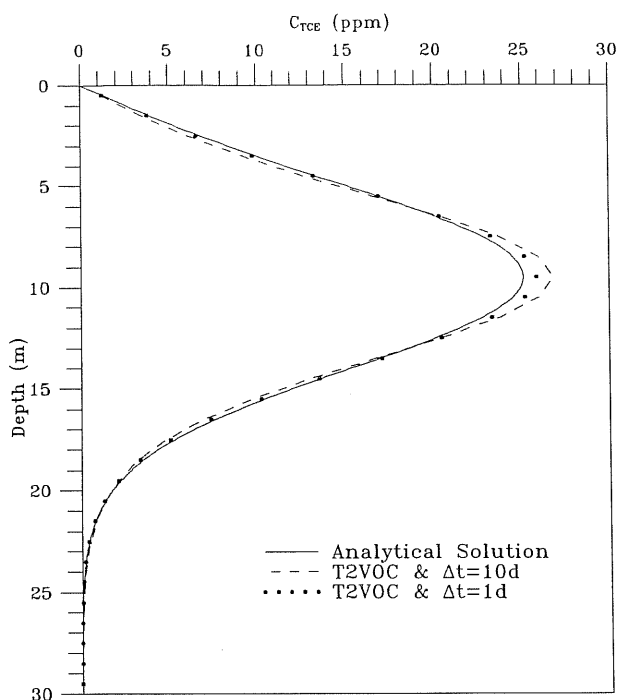
Fig. 4a   Comparison of calculated TCE concentrations in the aqueous phase at t = 100d (constant $\Delta z = 1m$)
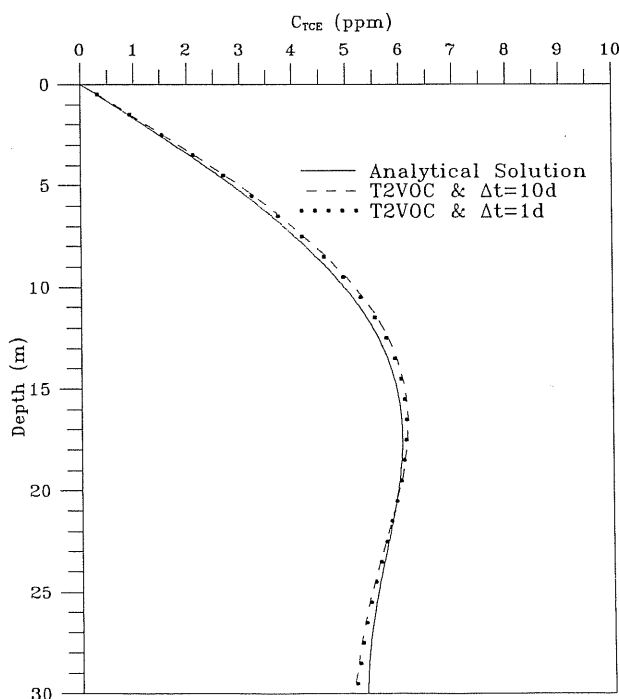

Fig. 4b   Comparison of calculated TCE concentrations in the aqueous phase at t = 1000d (constant $\Delta z = 1m$)

were conducted using two different uniform time steps, i.e., $\Delta t = 1d$ and $\Delta t = 10d$. The TCE concentration in the aqueous phase at the end of 100d and 1000d for different cases are plotted in Figures 3a and 3b ($\Delta z = 0.1m$), and Figures 4a and 4b ($\Delta z = 1m$). These results are compared with the corresponding analytical solutions.

A thoughtful comparison among these figures gives us the following conclusions: (a) T2VOC results match the analytical solutions very well, (b) a reasonably large time step can give a result that is almost as good as that offered by a small time step, particularly as time increases, (c) a reasonably large grid size can give a result that is almost as good as that offered by a small grid size except for a possible loss of some detail information at places with big changes. Comparing Figures 4b with 3b, one could find that the discrepancy between the T2VOC solution and the analytical solution at the water table is missing from Figure 4b due to its large grid size. As previously mentioned, the large and non-uniform moisture content right above the water table (Figure 2) has been approximated to a small value in the analytical solution, which overestimates the gas-filled porosity and the gas diffusion above the water table. However, the large discrepancy appears only at times when the contamination front reaches the water table (e.g., at $t = 1000d$ rather than $t = 100d$). The interesting finding from Figure 3b is also an example demonstrating the strong capability of a numerical code such as T2VOC in modeling the real problem.

Acknowledgement

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