Comparison of CXTFIT and Hydrus-1D projects

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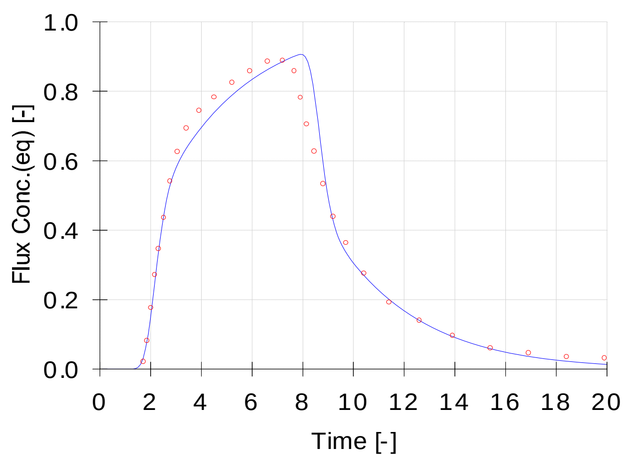
Comparing results of CXTFIT and HYDRUS-1D calculations is not always straightforward as both programs are using different units. While users of CXTFIT often use dimensionless variables, users of HYDRUS-1D are restricted to dimensional variables. We will demonstrate such comparison on the CZTFIT Fig79b project (Toride et al., 1995, page 98) and the HYDRUS-1D project (included). The Fig79b project is installed together with the STANMOD software package and is located in the Inverse workspace.

In this example a pulse of boron tracer was applied for T_2=6.964 pore volumes to the 30-cm long column as used in another example presented in Figure 7.9a of Toride et al. (1995) [Exp. 3-1 of van Genuchten, 1974]. The estimated parameters were v = 38.5 cm d^{-1} and R = 3.9 (K_d = 1.04 g^{-1}cm^3, ρ = 1.222 gcm^{-3}, and θ = 0.445). Figure below shows observed and fitted BTCs with optiomized parameters β = 0.578 and ω = 0.7. Substituting θ_m/θ = 0.822, as obtained from previous experiment, into the expression for β yields f = 0.49 for the fraction of sorption sites in contact with the mobile phase.



Toride, N., F. J. Leij, and M. Th. van Genuchten, The CXTFIT code for estimating transport parameters from laboratory or field tracer experiments. Version 2.0, *Research Report No. 137*, U. S. Salinity Laboratory, USDA, ARS, Riverside, CA, 1995.

van Genuchten, M. Th., Mass transfer studies in sorbing porous media, Ph. D. thesis, New Mexico State Univ., Las Cruces, New Mexico, 1974.

Mathematical Model: Physical Nonequilibrium Transport Model

Governing Equations:

$$\theta_m \frac{\partial c_m}{\partial t} + f\rho \frac{\partial s_m}{\partial t} + \theta_{im} \frac{\partial c_{im}}{\partial t} + (1-f)\rho \frac{\partial s_{im}}{\partial t} = \theta_m D \frac{\partial^2 c_m}{\partial x^2} - \theta_m v_m \frac{\partial c_m}{\partial x}$$

$$\theta_{im} \frac{\partial c_{im}}{\partial t} + (1-f)\rho \frac{\partial s_{im}}{\partial t} = \alpha\left(c_m - c_{im}\right)$$

$$s = kc \qquad v_m = \frac{q}{\theta_m} \qquad \theta = \theta_m + \theta_{im} \qquad \phi_m = \frac{\theta_m}{\theta} \qquad S = fS_m + (1-f)S_{im}$$

Initial condition:

$$c_m(x,0) = c_{im}(x,0) = c_i$$

Boundary conditions:

$$-D\frac{\partial c_m}{\partial x} + v_m c_m = vc_0 \qquad x = 0$$

$$\frac{\partial c_m}{\partial x} = 0 \qquad x = \infty$$

Dimensionless variables:

$$T = \frac{vt}{L} = \frac{v_m t \phi_m}{L} \qquad Z = \frac{x}{L} \qquad P = \frac{v_m L}{D} \qquad C_1 = \frac{c_m - c_i}{c_0 - c_i} \qquad C_2 = \frac{c_{im} - c_i}{c_0 - c_i}$$

$$R = 1 + \frac{\rho k}{\theta} \qquad R_m = 1 + \frac{f\rho k}{\theta_m} \qquad \omega = \frac{\alpha L}{\theta_m v_m} \qquad \beta = \frac{\theta_m + f\rho k}{\theta + \rho k} = \frac{\theta_m R_m}{\theta R}$$

Dimensionless system:

$$\beta R \frac{\partial C_1}{\partial T} + (1-\beta) R \frac{\partial C_2}{\partial T} = \frac{1}{P}\frac{\partial^2 C_1}{\partial Z^2} - \frac{\partial C_1}{\partial Z}$$

$$(1-\beta) R \frac{\partial C_2}{\partial T} = \omega(C_1 - C_2)$$

Boundary conditions:

$$-\frac{1}{P}\frac{\partial C_1}{\partial Z} + C_1 = 1 \qquad Z = 0$$

$$\frac{\partial C_1}{\partial Z} = 0 \qquad Z = \infty$$

Summary of Parameters Used in CXTFIT:

v = 38.5 cm d^{-1}
D = 15.5 $cm^2 d^{-1}$
R = 3.9 (= $1+ K_d\rho/\theta$ = 1+1.04 * 1.222 / 0.445 = 3.86) (dimensionless)
L = 30 cm
T_0 = 6.494 (dimensionless)
β = 0.578 (fitted)
ω = 0.7 (fitted)
Actual physical parameters from which R and v are calculated
K_d = 1.04 $g^{-1}cm^3$
ρ = 1.222 gcm^{-3}
θ = 0.445
θ_m = 0.822θ

Summary of Parameters Used in HYDRUS-1D:

q = 17.13 cmd^{-1} (= $v\theta$ = 38.5 *0.445)
θ_m = 0.366 (= 0.445*0.822)
θ_{im} = 0.079 (= $\theta - \theta_m$ = 0.445-0.366)
α = 0.4 (= $\omega\theta v/L$ = 0.7*0.445*38.5/30)
f = 0.491 (= $[\beta(\theta+\rho K_d)-\theta_m]/\rho K_d$) = [0.578(0.445+1.222*1.04)-0.366]/1.222*1.04)
$t = TL/v = 0.7792T$
t_0 = 5.06 d (= tT_0 = 0.7792*6.494)

Figure below shows observed and calculated BTCs with HYDRUS-1D using the parameters evaluated above. One can see that correspondence between HYDRUS-1D and CXTFIT is perfect.