CXTFIT/Excel, A Data Analysis Tool for Tracer Experiments, is Available Online Now

CXTFIT/Excel: A Data Analysis Tool for Transport Experiments

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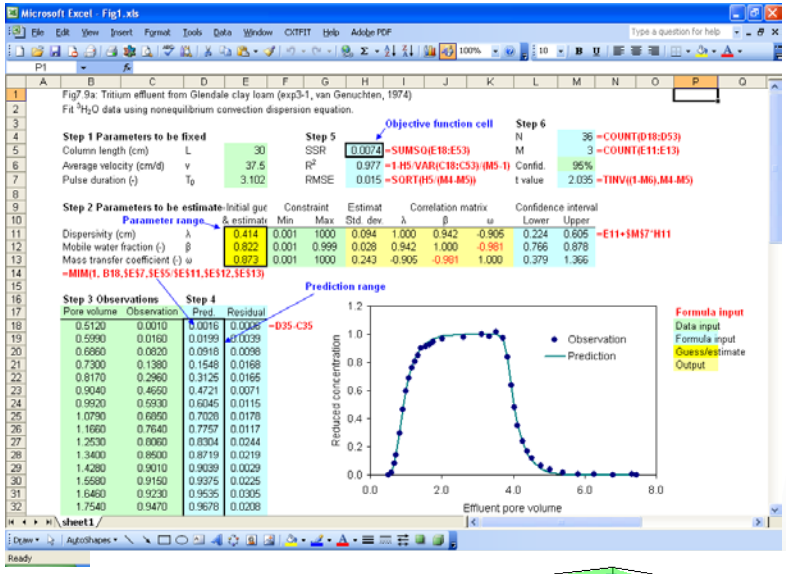
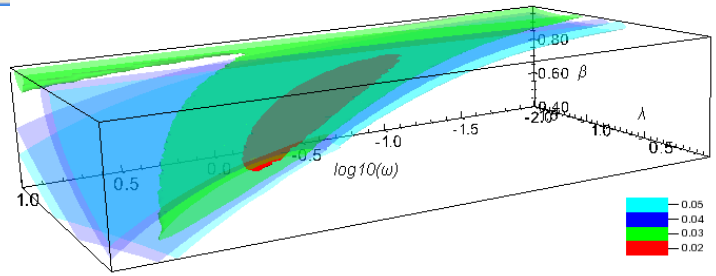
Example of intact soil column used in transport experiments.

- Coupled hydrological, biological, and geochemical processes that influence the fate of contaminants in the subsurface are studied by transport experiments on laboratory soil columns and in field plots.
- Different models may match observations equally well. A systematic method using sensitivity and uncertainty analysis is presented to evaluate models and parameters, and understand and quantify the processes.
- Functions for solving 1-D equilibrium and nonequilibrium convection dispersion equations, and macros for optimization, sensitivity/uncertainty and Monte Carlo analysis were coded in VBA for use in Excel.
- With CXTFIT/Excel, any parameter can be estimated and its sensitivity and uncertainty values are quantified. Concentration-dependent analytical errors and prior parameter information are incorporated into weighted least squares with penalty function for data analysis.
- The model can be used by researchers to better understand and quantify coupled processes influencing the transport and fate of contaminants at DOE sites.





Response surface of the root mean squared error (RMSE) shows parameter uncertainty

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Needs: Soil column and field-scale experiments are conducted to investigate the coupled hydrological, geochemical, and biological processes that govern contaminant fate and transport. Interpretation of these experimental data is challenging due to uncertainty in experimental conditions and correlations among multiple transport mechanisms.

Technical Approach: We coded the analytical solutions for one-dimensional equilibrium and nonequilibrium convection equations as Microsoft® Visual Basic for Applications® functions. Macros for optimization, sensitivity analysis, parameter uncertainty analysis, error propagation, response surface calculation, and Monte Carlo analysis were developed with user-friendly interfaces. With CXTFIT/Excel, any parameter can be estimated with sensitivity and uncertainty quantification; observation uncertainty and prior information can be incorporated into weighted least squares with penalty. The code was verified against CXTFIT 2.0 and was demonstrated on soil column experiments, DNAPL model calibration, pump tests, and two-well tests .

Future Applications: CXTFIT/Excel can be used to analyze traditional column and plot-scale experimental data, as well as for the analysis of complex long-term experiments using multiple tracers and particles. This type of data analysis can contribute to a better understanding of the coupled processes influencing the transport and fate of contaminants at DOE sites.

References:

Tang, G., Mayes, M. A., Parker, J. C., Yin, X. L., Watson, D. B. and Jardine, P. M. 2009. Improving parameter estimation for column experiments by multi-model evaluation and comparison. *Journal of Hydrology* 376, 567–578. doi:10.1016/j.jhydrol.2009.07.063.

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