1DTempPro V2:

New Features for Inferring Groundwater/Surface-Water Exchange

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ABSTRACT

A new version of the computer program 1DTempPro extends the original code to include new capabilities for (1) automated parameter estimation, (2) layer heterogeneity, and (3) time-varying specific discharge. The code serves as an interface to the U.S. Geological Survey model VS2DH and supports analysis of vertical one-dimensional temperature profiles under saturated flow conditions to assess groundwater/surface-water exchange and estimate hydraulic conductivity for cases where hydraulic head is known.

Introduction

The computer program 1DTempPro (Voytek, et al., 2013) was introduced to aid in the analysis of one-dimensional (1D) vertical temperature profiles to infer rates of vertical groundwater/surface-water exchange. The program provided an easy-to-use graphical user interface (GUI) that ran VS2DH (Healy and Ronan, 1996). The GUI facilitated calibration of coupled numerical heat-transport and groundwater flow models to measured temperature time series within saturated sediments. Such analysis has become common in hydrologic investigations, and the interested reader is referred to reviews by Constantz (2008), Anderson (2005), and Constantz and Stonestrom (2003), and the seminal study of Lapham (1989). Although interfaces were developed previously (Swanson and Cardenas, 2011; Gordon et al., 2012) for analytical methods (e.g., Stallman, 1965; Keery et al., 2007; and Hatch et al., 2006), 1DTempPro represented the first GUI to capitalize on the flexibility afforded by numerical models. Since publication, the code has been used in a number of studies (e.g., Briggs et al., 2013; Briggs et al., 2014). A schematic of the measurement procedure and model construction is given in Figure 1.

The original version of 1DTempPro had several simplifications that limited its utility. First, the code supported only manual calibration, which required trial-and-error adjustment by the user and did not allow for quantitative error assessment of the final result. Second, Version 1 only allowed for uniform physical properties; i.e., layer heterogeneity was not supported. Third, the only options for constraining
hydraulic boundary conditions were constant specific discharge, constant head, or time-varying head if the user had the measurements available. The user was unable to input time-varying specific discharge and evaluate the resulting effect. The purpose of this Methods Note is to introduce Version 2 of 1DTempPro, which overcomes these limitations.

**Approach**

Version 2 of 1DTempPro offers all the functionality of Version 1 (Voytek, et al., 2013) and maintains similarity and backward compatibility to allow a seamless transition for experienced users. The GUI serves as a pre- and post-processor to VS2DH designed to streamline construction and calibration of models to 1D vertical temperature data. Major additions in Version 2 include new features for (1) parameter estimation, (2) layer heterogeneity, and (3) time-varying specific discharge. Figure 1 outlines these new features and how they fit into the original program’s work flow. The modified workflow supports two modes of analysis: solving for hydraulic conductivity, $K$, and solving for specific discharge, $q$. Figure 2 shows a screenshot of the new GUI.

**Parameter estimation**

Parameter-estimation tools are used increasingly in hydrologic modeling to help identify optimal parameters and rigorously measure estimation uncertainty (Hill and Tiedeman, 2007). Once data are loaded and initial model parameterization is complete, the user can have 1DTempPro V2’s parameter-estimation tools automatically find individual best-fit parameter values. Parameter estimation is implemented using iterative Levenberg-Marquardt nonlinear regression to find the value that minimizes the sum of squared residuals between predicted and observed temperatures (Levenberg, 1944; Marquardt, 1963). The user may choose to estimate $q$, $K$, porosity, thermal conductivity, or sediment heat capacity. With the exception of discharge, all other parameters must remain positive; hence for these parameters, the estimation procedure is implemented for the natural logarithm of the parameter value to prevent unrealistic negative values.
The user can select between several termination conditions for the parameter-estimation procedure including a maximum number of iterations, a minimum absolute change of the sum of squares between iterations, or a minimum relative change of the parameter value between iterations. Values for these termination criteria can be modified from default values within the 1DTempPro V2 software.

For ease of use, 1DTempPro V2 allows for estimation of only one parameter at a time. In principle, it is possible to estimate multiple physical parameters simultaneously; however, reliable estimation requires that parameters are not correlated, and thus estimation of multiple parameters requires additional analysis of correlation and sensitivity. Users requiring such analyses can link VS2DH with PEST (Doherty, 2010) or UCODE (Poeter et al., 2005).

Most users of 1DTempPro V2 will focus analysis on \( q \) or \( K \) due to the potential for non-unique simulations resulting from multiple thermal parameter combinations. The user may be able to estimate multiple parameters sequentially, but such analyses should be performed with caution. The values of fixed parameters must be known accurately to ensure robust estimation using a sequential approach. We strongly recommend that the user initiate parameter estimation based on a starting model identified by direct measurements of sediment thermal properties, estimations based on the guidance provided by Lapham et al. (1989), and further manual calibration. This will lead to a more robust optimization because the user will have insight to the non-uniqueness of various models arising from correlation between and sensitivity to the different parameters.

1DTempPro V2 supports limited analysis of parameter uncertainty. The posterior covariance matrix for the parameter-estimation problem is calculated as

\[
\mathbf{C} = (\mathbf{J}^T \mathbf{W}^{-1} \mathbf{J})^{-1},
\]

where \( \mathbf{J} \) is the Jacobian with elements \( \frac{\partial T_i}{\partial p_j} \), given by the sensitivity of each temperature observation, \( T_i \), with respect to each parameter, \( p_j \), and \( \mathbf{W} \) is a diagonal weighting matrix, with elements \( W_{ii} \) given by the
temperature measurement variance, $\sigma_{T,i}^2$. Because we only vary one parameter at a time and assume all temperature measurements have uniform error, $\sigma_{T}^2$, this equation reduces to

$$\sigma_p^2 = \sigma_T^2 \sum_i \left( \frac{\partial T_i}{\partial p} \right)^{-2},$$

where $\sigma_p^2$ is the estimation variance associated with the individual parameter being optimized, $p$. When estimating the logarithm of a parameter, an additional step is taken to convert the optimized log parameter, $\ln(p)$, and variance, $\sigma_{\ln(p)}^2$, back to the unlogged parameter, $p$, and variance, $\sigma_p^2$:

$$p = e^{(\ln(p) + \frac{\sigma_{\ln(p)}^2}{2})}, \text{ and}$$

$$\sigma_p^2 = e^{(2\ln(p) + \sigma_{\ln(p)}^2)} (e^{\sigma_{\ln(p)}^2} - 1).$$

Reporting the standard estimation error $\sigma_p$ provides the user with an idea of how sensitive the data fit is to that parameter value. When performing parameter estimation, 1DTempPro V2 produces additional output files summarizing progress of the parameter estimation procedure at each iteration and a detailed report of the initial and final parameters. These files facilitate archiving and reproduction of calibration results.

Layer heterogeneity

1DTempPro V2 allows users to input different physical properties for multiple model layers, expanding the potential applications of the code to more realistic geologic situations, e.g., systems where the streambed is armored or multiple layers have been identified by coring. As the layer geometry is constructed, the GUI displays layer divisions and measurement locations, visible in Figure 2. Layer boundaries are adjusted to match the discretization of the finite-difference model, which can be adjusted in the advanced options. Additionally, the number of layers is limited to 10 to ease graphical manipulation of layer boundaries. A new output file is generated that records the input layer geometry. An example dataset to demonstrate 1DTempPro’s new layer capabilities is included with the software distribution.
When multiple layer geometry is specified, only estimation of specific discharge is allowed because it is a property of the entire system. Although estimation of other layer-specific parameters is possible in principle, issues of parameter correlation and non-uniqueness are likely. The simple tools available in 1DTempPro V2 are not designed for evaluating parameter correlation and non-uniqueness. Again, the interested user can link VS2DH to UCODE or PEST for such analyses.

**Time-varying specific discharge**

The analysis procedure of 1DTempPro Version 1 assumed that fluid flux was constant in time, or varied according to a known, user-supplied variation of hydraulic head. Version 2 allows for time-varying flux and provides a simple graphical tool for the user to adjust the specific discharge with time. Alternatively, 1DTempPro can now read in a time-series of time-varying flux. This is useful if the entire span of the dataset cannot be fit with a single specific discharge and head data are unavailable. The graphical implementation makes small adjustments simple. The time-varying specific discharge is saved in the archive folder, so the user has reference to any changes made graphically. Note that parameter estimation for time-varying $q$ is not supported.

**Example Dataset: Time-varying discharge from fence installation**

To illustrate new capabilities of the GUI, we process a dataset from a shallow vertical profile in the streambed of the Quashnet River (see Briggs et al., 2014 for additional detail). Streambed temperature was measured at depths of 0.01, 0.04, and 0.07 m in a zone of known groundwater upwelling. After 6 days of ambient data collection, a semi-permeable fence was installed part way across the stream, diverting and focusing flow and increasing hydraulic pressure on the streambed in the area of the vertical profile. Installation of the fence resulted in a change from weak groundwater upwelling, or negative specific discharge, to strong downwelling, or positive specific discharge (Figure 3a).

Thermal properties (i.e., thermal conductivity, sediment heat capacity, and effective thermal diffusivity) of the streambed were measured using KD2-Pro instrument (Decagon Devices, Pullman, WA).
An initial model for temporally-variable specific discharge was estimated analytically at 2-hr increments by modeling the vertical propagation of diurnal temperature signals using the VFLUX program (Gordon et al., 2012). Using this time-varying specific discharge as our hydraulic constraint and the 0.01 and 0.07 m temperature series as boundary conditions, we ran 1DTempPro V2 to see how well the model fit the data. The simulation fit the 0.04-m temperature data well overall (RMS=0.13 °C, Figure 3b), but there was a notable misfit directly following fence installation. Transitions in specific discharge modeled analytically using VFLUX may show a lag of several signal periods compared to data when fluid flux changes instantaneously (Lautz, 2012), as we may have expected after fence installation.

Here, we use 1DTempPro V2 to find a better fit to the specific discharge immediately after fence installation. To do this, we consider only data following the fence installation and determine \( q \) using the new parameter estimation functionality of 1DTempPro V2 (Figure 3c). The Levenberg-Marquardt algorithm converged at a downward \( q \) estimate of 1.56 +/- 0.06 md\(^{-1}\) after two iterations based on the default termination conditions. Finally, the original specific discharge time series was modified to use this optimized value after the fence installation (Figure 3a). The resulting model from 1DTempPro V2 fit the 0.04-m data better than before with a total RMS of 0.08 °C, comparable to the sensor precision of 0.06 °C (Figure 3d). This example highlights the new time-varying discharge and parameter estimation functionality of 1DTempPro V2, and illustrates a major strength of the numerical approach in that actual fits to temperature data can be evaluated, which is not done with the analytical models.

**Discussion & Conclusions**

1DTempPro Version 2 extends the original code to include capabilities for parameter estimation, layer heterogeneity, and time-varying exchange, further capitalizing on the capabilities of the underlying numerical model, VS2DH. This new version greatly expands the range of problems for which 1DTempPro V2 is applicable. Possible future extensions include functionality to (1) estimate multiple...
parameters simultaneously, (2) model 2D flow and heat-transport, and (3) allow for variably saturated conditions and analysis of data from ephemeral streams or tidal areas. The 1DTempPro V2 code was written following object-oriented paradigm in C# to foster extensibility and future development.

Supporting Information

Supplemental material available online includes the 1DTempPro V2 installation, which also can be downloaded from http://water.usgs.gov/ogw/bgas/1dtemppro/, and README and TUTORIAL files with information for installation, troubleshooting, and examples of code operation.

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References


Levenberg, K. 1944 A method for the solution of certain nonlinear problems in least squares, Quarterly of Applied Mathematics, 4: 164-168


Figure 1. (a) A schematic of data collection including a temperature probe with four sensors (colored dots) and a pair of piezometers, installed in a 3-layer streambed; (b) measurements of temperature (T), head difference ($\Delta h = h_1 - h_2$) or q forcing for boundary conditions; (c) numerical model consisting of a single column of fully saturated finite-difference cells with layer-dependent properties; (d) comparison of modeled and observed data; and (e) optional automated parameter-estimation procedure, which involves minimizing the sum of the squared errors (SSE) by iteratively updating a selected system parameter and rerunning the model.
Figure 2. Main window of the 1DTempPro V2 interface. The left panel allows for input of model parameters, including geometry, physical properties, and hydrologic constraints. The model geometry is displayed in the center column, and time-varying hydrologic constraints are displayed in the bottom right. The top right plot compares simulated temperatures to measured data. Tools for parameter estimation are accessed under the Options menu.
Figure 3. Demonstration of 1DTempPro V2’s new capabilities, including time-varying specific discharge and parameter estimation. (a) Analytical estimate for specific discharge (black), and modification based on 1DTempPro V2 optimization (green). Positive discharge indicates upwelling and negative discharge downwelling. (b) 1DTempPro V2 simulation results using specific discharge time series calculated analytically (black line in (a)); the simulation accurately reproduces early time data but there is some misfit after the fence was installed. (c) Simulation results of post-fence-installation temperature data using optimized $q$ value (green line in (a)). (d) Simulation results with analytical $q$ estimate before fence installation and 1DTempPro V2 estimate after installation. There is reduced misfit compared to (b). Note that output from 1DTempPro was exported to prepare this figure outside the GUI.