1DTempPro Known Issues through v. 1.0.1.2

Created July 29, 2014; updated August 5, 2014

1DTempPro offers two modes of use: (1) manual calibration of a flow and heat-transport model to identify specific discharge (q), and (2) manual calibration of a flow and heat-transport model to identify hydraulic conductivity, K, if head data are available. A bug has been discovered in the code affecting reported results for mode (1); this bug does not affect results from analysis in mode (2).

The value of q used in the simulation may not exactly match the value specified by the user. The discrepancy depends on the departure of simulated temperatures from 20°C. In its current form, for mode (1), the code uses specified head boundary conditions and a combination of K and head gradient that reproduce the entered q under Darcy's Law; however, this approach does not properly account for the temperature dependence of K in the VS2DH code. In VS2DH, the K input is for a reference K at 20°C. The K used in the VS2DH code is modified per the temperature dependence of the viscosity of water. Thus, the simulated q may not exactly match the entered q, particularly when the model domain deviates strongly from 20°C. **Table 1** provides an evaluation of the magnitude of errors for scenarios with varying temperature deviation from 20°C at the bottom boundary.

A corrected 1DTempPro code (version 1.2.0.2) was posted on this web site on August 5, 2014.

For a short-term fix in previous versions, we advise the user to inspect the VS2DH output file (vs2dh.out), which is archived by 1DTempPro. The simulated q can be easily found by searching the file for the text string "FLUX INTO DOMAIN ACROSS SPECIFIED PRESSURE HEAD BOUNDARIES" and selecting the value in the third column (**Figure 1**). This flux will not have a directionality (- or +, for upwelling or downwelling, respectively) associated with it, but directionality is defined by the original GUI input. Note that although the flow problem is solved as a steady-state condition, K can vary between time steps according to the temperature profile, and thus q also may vary. Flux is calculated at every time step and reported in the output file. For most problems, temporal variation of q should be small, unless temperature changes are very large.

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---------- MASS BALANCE SUMMARY FOR TIME STEP     5136 ----------
    RECHARGE PERIOD NUMBER      1284
    TOTAL ELAPSED SIMULATION TIME =   7.703990E+05 SEC

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+                                                                                                                                          +
+                                                                                 TOTAL THIS          RATE THIS                        +
+                              VOLUMETRIC FLOW BALANCE                   TOTAL     TIME STEP          TIME STEP                        +
+                                                                       M   **3      M   **3          M   **3/SEC                       +
+    FLUX INTO DOMAIN ACROSS SPECIFIED PRESSURE HEAD BOUNDARIES --     9.58627E+00   9.36310E-04      1.25108E-05                       +
+  FLUX OUT OF DOMAIN ACROSS SPECIFIED PRESSURE HEAD BOUNDARIES --    -9.58858E+00  -9.36309E-04     -1.25108E-05                       +
+             FLUX INTO DOMAIN ACROSS SPECIFIED FLUX BOUNDARIES --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+           FLUX OUT OF DOMAIN ACROSS SPECIFIED FLUX BOUNDARIES --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                     TOTAL FLUX INTO DOMAIN --      9.58627E+00   9.36310E-04      1.25108E-05                       +
+                                   TOTAL FLUX OUT OF DOMAIN --     -9.58858E+00  -9.36309E-04     -1.25108E-05                       +
+                                                EVAPORATION --      0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                               TRANSPIRATION --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                   TOTAL EVAPOTRANSPIRATION --      0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                 FLUID FROM BOUNDARY CHANGE  --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+                            CHANGE IN FLUID STORED IN DOMAIN --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                       FLUID VOLUME BALANCE --     -2.30350E-03   4.49385E-10      6.00461E-12                       +
+                                                                                                                                          +
+                                                                                                                                          +
+                                 ENERGY MASS BALANCE                                                                                      +
+                                                                          J              J              J   /SEC                        +
+    FLUX INTO DOMAIN ACROSS SPECIFIED PRESSURE HEAD BOUNDARIES --     4.65367E+08   4.57390E+04      6.11158E+02                       +
+  FLUX OUT OF DOMAIN ACROSS SPECIFIED PRESSURE HEAD BOUNDARIES --    -6.15617E+08  -6.20948E+04     -8.29701E+02                       +
+             FLUX INTO DOMAIN ACROSS SPECIFIED FLUX BOUNDARIES --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+           FLUX OUT OF DOMAIN ACROSS SPECIFIED FLUX BOUNDARIES --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                     CONDUCTIVE FLUX INTO DOMAIN --     1.60144E+08   1.73203E+04      2.31430E+02                       +
+                                   CONDUCTIVE FLUX OUT OF DOMAIN --    -9.93748E+06  -1.10090E+03     -1.47100E+01                       +
+                                     TOTAL FLUX INTO DOMAIN --      6.25511E+08   6.30593E+04      8.42588E+02                       +
+                                   TOTAL FLUX OUT OF DOMAIN --     -6.25554E+08  -6.31957E+04     -8.44411E+02                       +
+                                   TOTAL EVAPOTRANSPIRATION --      0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                          FIRST ORDER DECAY --      0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                    ADSORPTION/ION EXCHANGE --      0.00000E+00   0.00000E+00      0.00000E+00                       +
+                                 ENERGY FROM BOUNDARY CHANGE --     0.00000E+00   0.00000E+00      0.00000E+00                       +
+                            CHANGE IN ENERGY STORED IN DOMAIN --    -1.77676E+04  -8.86750E+01     -1.18486E+00                       +
+                                       ENERGY MASS BALANCE --      -2.55299E+04  -4.77550E+01     -6.38094E-01                       +
+                                                                                                                                          +
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Figure 1. Example output file showing where specific discharge is found.

Table 1. For these synthetic examples, all 1DTempPro models were setup through the GUI window to be 0.5 m in vertical extent, upper boundary temperature as a pure sin wave (mean 20°C, amplitude 4°C, period 1 day), observation point at 0.07 m, and upwelling flux at -1.73×10^{-5} ms^{-1}. The bottom boundary was shifted progressively colder to simulate the effect of a stronger mean thermal gradient between surface water and groundwater, as may be expected in summer. Discrepencies between the user entered flux and actual model flux range from 0% for the 20°C model domain to 31% when groundwater temp is 5°C.

Surface-water mean temp (°C)	Groundwater temp (°C)	user entered flux (ms^{-1})	actual model flux (ms^{-1})	percent difference (%)
20	20	1.73×10^{-5}	1.73×10^{-5}	0
20	15	1.73×10^{-5}	1.55×10^{-5}	10
20	10	1.73×10^{-5}	1.36×10^{-5}	21
20	5	1.73×10^{-5}	1.20×10^{-5}	31