Supplementary Materials Document S1 for Wiebe, A.J., and Rudolph, D.L., *Meteorological and hydrological data from the Alder Creek watershed, SW Ontario*

# GNU Octave code and PEST file formats employed for vadose zone drainage calculations

**Introduction**

This supplementary document contains the code and file formats used to run the Stallman (1965) temperature analysis used to estimate vadose zone drainage rates. Filenames are in bold headings; code or text within files is written in regular font. One table that summarizes the parameters in the PEST (Doherty, 2015) *.pst* file is included under the heading *PEST parameters*. Each file or table is listed under its own heading in this document. Comments in the GNU Octave (Eaton et al., 2019) scripts are preceded by the "%" symbol, and lines beginning with this symbol and carrying over to the next line should be interpreted as occurring on a single line in the *.m* file. An ellipsis ("...") is used in the PEST *.ins* and *.pst* files to indicate lines of text following the same pattern as those given above. For example, the ellipses in the *.pst* file indicate that the omitted lines follow the pattern of a label with an incrementally increasing number, a daily average temperature value derived from the Wiebe et al. (2019) dataset, a weight, and the observation group along the line, similar to the previous two lines and the immediately following line. The temperature data used as the observations were the daily averages from the CS109 sensors for the time period 1 Dec 2014 to 30 Oct 2017 (Wiebe et al., 2019). Table S1.1 lists the PEST parameter names along with the variables. The file "stallmanIn3.txt" is the input file that PEST modifies prior to running the script "runstallman3.m" via the Windows batch file "runstallman3.bat".

**runstallman3.m**

```
% runstallman3.m
%
% Andrew J. Wiebe, 28 Oct 2021
%
% Octave-5.1.0.0 Script
%
% Use the Stallman (1965) method to estimate temperatures beneath a losing stream reach or DFR site at a given depth
%
% Set up to run with PEST!

% parameters to modify
% To          = c(1); % 10 deg C
% deltaT      = c(2); % 10 deg C
% q           = c(3); % 1E-6 m/s (estimate)
% offset      = c(4); % -5 (estimate)

% consts:
% C_b         = consts(1); % 2.84E6 J/m3/degC
% Kappa_b     = consts(2); % 2.0 J/m/s/degC
% Tau         = consts(3); % 365 * 24 * 60 * 60 s
% C_w         = consts(4); % 4.174E6 J/m3/degC, following Palmer et al. (1992)

output_precision(8);

consts = [2.84E6, 2.0, (365*24*60*60), 4.174E6]; % vector of constants

c = dlmread("stallmanIn3.txt", "\t",0,0);
c = c'
t = (0:1064)';

obs = dlmread("temp_observations_CS109s.txt", " \t",1,0); % read in the daily averages, derived from Wiebe et al. (2019)

depth = [0.3; 0.56; 0.91; 1.27; 2.14]; % depths of the selected CS109 temperatures sensors

SSE = 0;

for i = 1:5
        temp = stallman1965z(t,c,depth(i,1),consts);
        filename = sprintf('temp_sim_depth%g.txt', i);
        save(filename, 'temp');

        SE = (obs(:,i) .- temp);

        SSE = SSE + sum(SE .* SE);
end

SSE
```

**stallman1965z.m**

```
% stallman1965z.m
function temp = stallman1965z(t, c, z, consts)
%
% Andrew J. Wiebe, 26 Mar 2021; modifies version from 5 Feb 2021
% Octave-5.1.0.0 Script
%
% Use the Stallman (1965) method to estimate temperatures beneath a losing stream reach or DFR site at a given depth
%
% Input parameters:
% t = list of date indices (from 0 to 1095), i.e., number of days, where there are three sets of annual cycles with different data
% c(1) = To, i.e., mean temperature in surface water (deg C)
% c(2) = deltaT, i.e., amplitude of surface water temperature fluctuation, as | max or min minus To | (deg C)
% c(3) = q, i.e., infiltration flux estimate (m/s)
% c(4) = offset, i.e., shift in days to align the simulated and observed peaks and troughs more accurately
% z    = depth of the temperature response (m)
% consts(1) = C_b, i.e., volumetric heat capacity of bulk soil (J/m3/degC)
% consts(2) = Kappa_b, i.e., bulk aquifer thermal conductivity (J/m/s/degC)
% consts(3) = Tau, i.e., period of analysis - one day or one year (s)
% consts(4) = C_w, i.e., volumetric heat capacity of water (J/m3/degC)

To      = c(1);
deltaT  = c(2);
q       = c(3);
offset  = c(4);

C_b     = consts(1);
Kappa_b = consts(2);
Tau     = consts(3);
C_w     = consts(4);

Kprime = pi()*C_b / (Kappa_b * Tau);
Vprime = q * C_w / (2 * Kappa_b);
```

```
a = sqrt(sqrt(power(Kprime,2)+power(Vprime,4)/4) + power(Vprime,2)/2) - Vprime;
b = sqrt(sqrt(power(Kprime,2)+power(Vprime,4)/4) - power(Vprime,2)/2);


secondsPerDay = 24*60*60;

for i = 1:length(t)
        timestamp = (t(i,1) + offset) * secondsPerDay;
        temp(i,1) = To + deltaT * exp(-a * z) * sin(2 * pi() * timestamp / Tau - b * z);
end
```

**stallman3.pst**

```
pcf
* control data
restart estimation
4        5325     3        0        5
1 5 single point  1        0        0
10 -3 0.3 0.01 10
3.0 3.0 0.001
0.1
30 0.005 5 4 0.005 4
1 1 1
* parameter groups
group1   relative 0.1 0.0001 switch 2.0 parabolic
group2   relative 0.001 0.0 switch 2.0 parabolic
group3    absolute 0.1 0.0001 switch 2.0 parabolic
* parameter data
To       none     relative 9.0        -20.0             20.0       group1  1.0     0.0     1
deltaT   none     relative 9.0        -20.0             20.0       group1  1.0     0.0     1
qflux    log      factor   0.000001   0.00000001157     0.00001    group2  1.0     0.0     1
Toffset  none     relative 200        0                 365.0      group3  1.0     0.0     1
* observation groups
depth1obs
depth2obs
depth3obs
depth4obs
depth5obs
* observation data
d1t1     3.9512   1        depth1obs
d1t2     2.5604   1        depth1obs
...
d1t1065 8.52      1        depth1obs
d2t1     4.6657   1        depth2obs
d2t2     4.6033   1        depth2obs
```

```
...
d2t1065 10.439  1       depth2obs
d3t1    6.1676  1       depth3obs
d3t2    6.2749  1       depth3obs
...
d3t1065 12.13   1       depth3obs
d4t1    3.5336  1       depth4obs
d4t2    3.7875  1       depth4obs
...
d4t1065 12.501  1       depth4obs
d5t1    3.5886  1       depth5obs
d5t2    4.9588  1       depth5obs
...
d5t1065 13.01   1       depth5obs
* model command line
runstallman3.bat
* model input/output
stallmanIn.tpl                  stallmanIn3.txt
temp_obs_depth1.ins             temp_sim_depth1.txt
temp_obs_depth2.ins             temp_sim_depth2.txt
temp_obs_depth3.ins             temp_sim_depth3.txt
temp_obs_depth4.ins             temp_sim_depth4.txt
temp_obs_depth5.ins             temp_sim_depth5.txt
```

## PEST parameters

**Table S1.1: Parameters (all-caps) used in PEST (stallman3.pst) for simulating the average vadose zone annual drainage rate in the base of the topographic depression at Mannheim using CS109 soil temperature data.**

| | | | | | | |
|---|---|---|---|---|---|---|
| RSTFLE | PESTMODE | | | | | |
| restart | estimation | | | | | |
| NPAR | NOBS | NPARGP | NPRIOR | NOBSGP | | |
| 4 | 5325 | 3 | 0 | 5 | | |
| NTPLFLE | NINSFLE | PRECIS | DPOINT | NUMCOM | JACFILE | MESSFILE |
| 1 | 5 | single | point | 1 | 0 | 0 |
| RLAMBDA1 | RLAMFAC | PHIRATSUF | PHIREDLAM | NUMLAM | | |
| 10 | -3 | 0.3 | 0.01 | 10 | | |
| RELPARMAX | FACPARMAX | FACORIG | | | | |
| 3.0 | 3.0 | 0.001 | | | | |
| PHIREDSWH | | | | | | |
| 0.01 | | | | | | |
| NOPTMAX | PHIREDSTP | NPHISTP | NPHINORED | RELPARSTP | NRELPAR | |
| 30 | 0.005 | 5 | 4 | 0.005 | 4 | |
| ICOV | ICOR | IEIG | | | | |
| 1 | 1 | 1 | | | | |
| PARGPNME1 | INCTYP | DERINC | DERINCLB | FORCEN | DERINCMUL | DERMTHD |
| group1 | relative | 0.1 | 0.0001 | switch | 2.0 | parabolic |
| PARGPNME2 | INCTYP | DERINC | DERINCLB | FORCEN | DERINCMUL | DERMTHD |
| group2 | relative | 0.001 | 0.0001 | switch | 2.0 | parabolic |
| PARGPNME3 | INCTYP | DERINC | DERINCLB | FORCEN | DERINCMUL | DERMTHD |
| group3 | absolute | 0.1 | 0.0001 | switch | 2.0 | parabolic |
| PARNME1 | PARTRANS | PARCHGLIM | PARVAL1 | PARLBND | PARUBND | PARGP* |
| To | none | relative | 9.0 | -20.0 | 20.0 | group1 |
| PARNME2 | PARTRANS | PARCHGLIM | PARVAL1 | PARLBND | PARUBND | PARGP* |
| deltaT | none | relative | 9.0 | -20.0 | 20.0 | group1 |
| PARNME3 | PARTRANS | PARCHGLIM | PARVAL1 | PARLBND | PARUBND | PARGP* |
| qflux | log | factor | 0.000001 | $1.157\times10^{-8}$ | 0.00001 | group2 |
| PARNME4 | PARTRANS | PARCHGLIM | PARVAL1 | PARLBND | PARUBND | PARGP* |
| Toffset | none | relative | 200 | 0 | 365.0 | group3 |

* SCALE = 1.0, OFFSET = 0, DERCOM = 1 for all four parameters

**stallmanIn.tpl**

```
ptf $
$To                  $
$deltaT             $
$qflux              $
$Toffset            $
```

**temp_obs_depth1.ins**

```
pif *
*# columns: 1*
l1      [d1t1]1:50
l1      [d1t2]1:50
...
l1      [d1t1065]1:50
```

**temp_obs_depth2.ins**

```
pif *
*# columns: 1*
l1          [d2t1]1:50
l1          [d2t2]1:50
...
l1          [d2t1065]1:50
```

**temp_obs_depth3.ins**

```
pif *
*# columns: 1*
l1        [d3t1]1:50
l1        [d3t2]1:50
...
l1        [d3t1065]1:50
```

**temp_obs_depth4.ins**

```
pif *
*# columns: 1*
l1		[d4t1]1:50
l1		[d4t2]1:50
...
l1		[d4t1065]1:50
```

**temp_obs_depth5.ins**

```
pif *
*# columns: 1*
l1          [d5t1]1:50
l1          [d5t2]1:50
...
l1          [d5t1065]1:50
```

**runstallman3.bat**

```
octave runstallman3.m
```

**stallmanIn3.txt**

| | |
|---|---|
| | 9.9923471E+00 |
| | 1.1445864E+01 |
| | 3.5093653E-08 |
| 250 | 2.1758757E+02 |