

McCallum Transient Seepage Calculator

McCallum, A.M., Andersen, M.S., Rau, G.C. and Acworth, R.I., 2012. A 1-D analytical method for estimating surface water–groundwater interactions and effective thermal diffusivity using temperature time-series. *Water Resources Research*, 48(11): W11532.

This notebook utilizes diurnal transient sediment temperature profile to estimate groundwater seepage flux. Users are encouraged to familiarize with the theory beforehand. The assumed parameters in the transient models were porosity (η), volumetric heat capacity of fluid (ρc_f), volumetric heat capacity of solid (ρc_s), thermal dispersivity (β), and the thermal conductivity of the saturated porous media (k).

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In [ ]: from numpy import mean, array, cos, sin, arctan, log, sqrt, linspace
import numpy as np
from math import pi
from scipy.optimize import curve_fit, OptimizeWarning, fsolve
import warnings

porosity = 0.60
heat_capacity = 4190000
heat_capacity_solid = 2000000
diffusivity = 'TODO'
conductivity = 0.84
beta = 0.001
shallow_mid_dist = 0.1
str_temp_time_to = ""7/12/2014 0:00,7/12/2014 1:00,7/12/2014 2:00,7/12/2014 3:00,7/12/2014 4:00,
7/12/2014 5:00,7/12/2014 6:00,7/12/2014 7:00,7/12/2014 8:00,7/12/2014 9:00,
7/12/2014 10:00,7/12/2014 11:00,7/12/2014 12:00,7/12/2014 13:00,7/12/2014 14:00,
7/12/2014 15:00,7/12/2014 16:00,7/12/2014 17:00,7/12/2014 18:00,7/12/2014 19:00,
7/12/2014 20:00,7/12/2014 21:00,7/12/2014 22:00,7/12/2014 23:00,7/13/2014 0:00,
str_temp_to = ""24.51,24.38,24.20,24.07,23.88,23.70,23.51,23.45,23.45,23.63,23.95,24.26,24.51,
24.70,24.82,24.88,24.88,24.88,24.76,24.63,24.51,24.45,24.32,24.20,24.13""
str_temp_time_tz = ""7/12/2014 0:00,7/12/2014 1:00,7/12/2014 2:00,7/12/2014 3:00,7/12/2014 4:00,
7/12/2014 5:00,7/12/2014 6:00,7/12/2014 7:00,7/12/2014 8:00,7/12/2014 9:00,
7/12/2014 10:00,7/12/2014 11:00,7/12/2014 12:00,7/12/2014 13:00,7/12/2014 14:00,
7/12/2014 15:00,7/12/2014 16:00,7/12/2014 17:00,7/12/2014 18:00,7/12/2014 19:00,
7/12/2014 20:00,7/12/2014 21:00,7/12/2014 22:00,7/12/2014 23:00,7/13/2014 0:00,
str_temp_tz = ""21.07,21.07,21.07,21.01,21.01,20.94,20.94,20.82,20.82,20.82,20.82,
20.82,20.88,20.88,20.94,20.94,21.01,21.01,21.07,21.07,21.07,21.07,21.01""
expected = 10.3008

In [ ]: def get_frequency(data):
    ""Derive the frequency to be used in the transient functions.""
    # Frequency is derived from the frequency of the data. Hourly is 1/24, every two hours might be 1/48
    # One of the examples given works well with frequency = 1/24
    # All the tests seem to utilize data from a 24 hour period, so the frequency might always be 1/24
    return 2 / (len(data) - 1)

def parse_csv_str(csv_str, data_type):
    ""
    Receiving a CSV string.

    This function ignores all newlines and tabs before parsing
    the data into arrays of type 'datetime' or 'float'.
    ""
    # Strip all special (newline, tab, etc.) characters.
    csv_str = csv_str.replace('\n', '')
    csv_str = csv_str.replace('\r', '')
    csv_str = csv_str.replace('\t', '')
    csv_str = csv_str.rstrip(',')

    # Split on commas
    if data_type == 'datetime':
        return csv_str.split(',')

    elif data_type == 'float':
        # Data type is numerical (float), so we need to parse each value
        csv_array = [float(x) for x in csv_str.split(',')]
        return csv_array
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        return csv_array

def transient_ydata_func(parms, a, b, c, d, e, f, g, h):
    """Solved to discover the optimal seepage parameters."""
    return (a * cos((parms[2] * 1) * pi * parms[0]) + b * sin((parms[2] * 1) * pi * parms[0]) +
            c * cos((parms[2] * 2) * pi * parms[0]) + d * sin((parms[2] * 2) * pi * parms[0]) +
            e * cos((parms[2] * 3) * pi * parms[0]) + f * sin((parms[2] * 3) * pi * parms[0]) +
            g * cos((parms[2] * 4) * pi * parms[0]) + h * sin((parms[2] * 4) * pi * parms[0]) + p

In [ ]: # Parse the time series strings into arrays of strings (dates) and floats (temperatures)
temp_time_to = parse_csv_str(str_temp_time_to, 'datetime')
temp_time_tz = parse_csv_str(str_temp_time_tz, 'datetime')

try:
    temp_to = parse_csv_str(str_temp_to, 'float')
    temp_tz = parse_csv_str(str_temp_tz, 'float')
except ValueError:
    print("Could not parse provided time series data. Please check your input.")

if len(temp_time_to) + len(temp_time_tz) + len(temp_to) + len(temp_tz) < 12 * 4:
    print("Not enough time series data provided. Please check your input. There must be at least 12 data points.")
elif len(temp_time_to) != len(temp_time_tz) or len(temp_time_tz) != len(temp_to) or len(temp_to) != len(temp_tz):
    print("Please check your input. The four time series inputs should have the same number of points.")

In [ ]: RN1 = len(temp_to)
RN2 = len(temp_tz)
RN3 = 15
RN4 = 15

for i in range(16, RN1, 1):
    if temp_to[i] - temp_to[0] <= 1:
        RN3 = RN3 + 1

for i in range(16, RN2, 1):
    if temp_tz[i] - temp_tz[0] <= 1:
        RN4 = RN4 + 1

RN5 = len(temp_to)
RN6 = len(temp_tz)

# Ao for To and Tz:
L15 = mean(temp_to)
L20 = mean(temp_tz)

frequency = get_frequency(temp_to)

# xdata = linspace(0, 24, 25)
xdata = linspace(0, len(temp_to) - 1, len(temp_to))

In [ ]: # https://stackoverflow.com/questions/31301017/catch-optimizewarning-as-an-exception
with warnings.catch_warnings():
    warnings.simplefilter("error", OptimizeWarning)
    try:
        A1B1_calculated, pcov = curve_fit(transient_ydata_func, [xdata, L15, frequency], temp_to)
        A2B2_calculated, pcov = curve_fit(transient_ydata_func, [xdata, L20, frequency], temp_tz)
    except OptimizeWarning:
        print("Covariance of the parameters can not be estimated.")
    except RuntimeError:
        print("Least-Squares minimization has failed.")

In [ ]: # Run McCallum method:
P = 1 # Period (days)

# calculate amplitude & phase angle of the shallow depth
A1 = A1B1_calculated[0]
B1 = A1B1_calculated[1]
Po = 0
Pz = 0

if A1 == 0:
    A1 = 1E-99
if B1 == 0:
    B1 = 1E-99

Ao = (A1 ** 2 + B1 ** 2) ** 0.5

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if A1 < 0:
    Po = arctan(B1 / A1) + pi
else:
    Po = arctan(B1 / A1)

# calculate amplitude & phase angle of the deeper depth
A2 = A2B2_calculated[0]
B2 = A2B2_calculated[1]

if A2 == 0:
    A2 = 1E-99
if B2 == 0:
    B2 = 1E-99

Az = (A2 ** 2 + B2 ** 2) ** 0.5
if A2 < 0:
    Pz = arctan(B2 / A2) + pi
else:
    Pz = arctan(B2 / A2)

# Calculate Amplitude ratio & phase shift
AR = Az / Ao
PS = (Pz - Po) / (2 * pi) # phase shift unit is "day"
# Needed to change from < to <= in the case of 0, which resulted in NaN.
if PS <= 0:
    PS = (2 * pi + Pz - Po) / (2 * pi)

# ***start McCallum (2012) calculation***
dz = shallow_mid_dist # depth
n = porosity # porosity
PfCf = heat_capacity # volumetric heat capacity of fluid
PsCs = heat_capacity_solid # volumetric heat capacity of solid
PC = n * PfCf + (1 - n) * PsCs # heat capacity of saturated media
r = PC / PfCf
LnAR = log(AR)

# thermal front velocity
v = dz * (P ** 2 * LnAR ** 2 - 4 * pi ** 2 * PS ** 2) / (
    PS * (16 * pi ** 4 * PS ** 4 + 8 * P ** 2 * pi ** 2 * PS ** 2 * LnAR ** 2 + P ** 4 * LnAR

# Darcy velocity (seepage flux)
qz = v * r
X12 = qz * 100 # in cm/day

# calculate De (effective thermal diffusivity)
De = (dz ** 2 * P ** 2 * LnAR * (4 * pi ** 2 * PS ** 2 - P ** 2 * LnAR ** 2)) / (
    PS * (P ** 2 * LnAR ** 2 + 4 * pi ** 2 * PS ** 2) * (P ** 2 * LnAR ** 2 - 4 * pi ** 2 * P

# 'calculate thermal conductivity k
Beta = beta
ke = (De - beta * abs(v)) * PC / 86400

print(f'Seepage:      {round(X12, 4)}')
print(f'Diffusivity:  {round(De, 4)}')
print(f'Conductivity: {round(ke, 4)}')

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In []: