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Hydrology and Earth System Sciences Discussions

Interactive comment on "Comparison of heat tracer models in the estimation of upward flux through streambed sediments" *by* M. Shanafield et al.

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This paper considers the estimation of vertical fluxes in streambeds by 1-D analysis of temperature data under conditions of upward water flow. In particular, the authors study the applicability of analytical solutions based on steady-state 1-D flow and either steady-state or sinusoidal boundary conditions. The first one is recalled the Bredehoeft and Papadopolus (1965) solution to Stallman's (1960) equation (BP), and the second one the Hatch et al. (2006) and Keery et al. (2007) methods (HK). The authors first discuss a numerical test case and then switch to field data, where they calibrated a

numerical model with time-varying boundary conditions.

1 General Comments

My overall impression is that the authors fit specific analytical solutions to (virtual) data in cases where they are not appropriate to begin with. While I know that the literature of stream-groundwater exchange includes many erroneous applications of analytical expressions I don't see a reason to continue that.

1.1 Underlying Analytical Expressions

I may remark that the following equations are not new by any means. I just recall them to clarify matters. Let's start with the convection-condution equation using the notation of the authors:

$$\frac{\partial T}{\partial t} + v_f \frac{\partial T}{\partial z} - K_e \frac{\partial^2 T}{\partial z^2} = 0 \tag{1}$$

with

$$v_f = \frac{\varrho_w c_w q_z}{\varrho c} \tag{2}$$

$$K_e = \frac{K}{\varrho c} + D_{hyd} \tag{3}$$

subject to boundary conditions that have a steady-state, and a time-periodic contribution:

$$T(0,t) = T_{avg} + A \cos\left(\frac{2\pi t}{P}\right) \tag{4}$$

$$\lim_{z \to \infty} T(z,t) = T_\infty \forall t \tag{5}$$

To simplify the analysis, I have replaced the fixed temperature at depth L, used by the authors according to BP, by an auxiliary condition at the infinite-depth limit, $z \to \infty$. This is to simplify the analysis of the sinusoidal data. Also, I have immediately switched to the thermal front velocity v_f and the effective thermal diffusivity K_e to simplify notation (which is the sum of the thermal diffusivity and the hydromechanic dispersion coefficient D_{hyd}). At this point, no assumption is made whether v_f is positive or negative. I have also chosen the time t such that the periodic boundary condition becomes a cosine rather than a sine. The analytical solution for this problem is:

$$\begin{aligned} T(z,t) &= T_\infty + (T_{avg} - T_\infty) \exp\left(\frac{(v_f - |v_f|)z}{2K_e}\right) \\ &+ A \exp\left(\frac{v_f z}{2K_e} - \frac{\sqrt{\sqrt{v_f^4 + \frac{64\pi^2 K_e^2}{P^2}} + v_f^2 2}}{2K_e} z\right) \cos\left(\frac{2\pi t}{P} - \frac{\sqrt{\sqrt{v_f^4 + \frac{64\pi^2 K_e^2}{P^2}} - v_f^2 2}}{2K_e} z\right) \end{aligned} \tag{6}$$

That is, the steady-state and diurnal contributions are additive. Of course, Eq. (6) is the sum of the two analytical expressions cited by the authors. Note that, if $v_f > 0$, the steady-state contribution becomes a constant if the lower boundary is chosen at the infinite limit, which is not the case in the BP solution.

Eq. (6) has been known for a long period of time (and can easily be extended to temperature signals of multiple frequencies). The most important assumption is that the coefficients v_f and K_e must not vary in time. Choosing the fixed-temperature boundary at $z \to \infty$ is not a principal problem, but the resulting expression for a different location of the boundary is ugly to read if one does not like complex expressions.

1.2 Main Criticisms

1. The authors consider cases in which steady-state and diurnal contributions are overlain. It does not make sense to use analytical solutions for either only steady-state or only sinusoidal boundary conditions in such cases. This becomes evident in the numerical example. The reported miss-fits indicate either systematic bias (in case of the spectral approach of HK) or temporal fluctuations (in case of the steady-state approach of BP). Of course, one has to separate the time-fluctuating and steady-state contributions when using either of the two approaches. In the field example, the authors implicitly remove the steady-state contribution when applying the amplitude-dampening approach. However, they don't try to make use of the combined, existing analytical solution.

2. The authors make wrong statements about underlying assumptions in the analytical expressions. A prominent example is that there would be a difference whether conductive flux is predominantly upwards or downwards. That is simply wrong. It is important whether convection is upwards or downwards; and it is important whether a mean temperature gradient exists. But the analytical expressions don't mind whether groundwater or stream water is cooler in average.

3. The key problem in the field application is temporal variability of flow. The head-differences fluctuate on time scales of days. The estimated travel time of temperature is also in the range of one day. Thus, any analysis assuming quasi steady-state flow must be flawed. This is the true difficulty of the appliction, but the problem is not posed that way. I highly recommend that the authors change their virtual toy problem to something similar: A test case in which flow is transient, in which "data" are attempted to be fitted with a solution based on steady-state flow.

4. A core difficulty in using either only the steady-state contribution, or only the amplitude dampening, or only the phase shift is that the temperature propagation

behavior depends on two coefficients: v_f and K_e. The effective thermal diffusivity K_e depends on hydromechanic dispersion, porosity, and the mineral composition of the streambed. These properties are not too well constrained. In particular the method based on steady-state heat transport yields exclusively the thermal Peclet number $v_f z/K_e$ rather than v_f (and thus q_z) itself. A combined analysis of all three components yields, at least in theory, a handle on both v_f and K_e.

2 Specific Comments

1. throughout the text: Replace "diel" with "diurnal".
2. throughout the text: There is no "flat" temperature, there is a constant one.
3. throughout the text: Use consistent notation including consistent choices when a velocity is positive or negative.
4. page 4306, lines 3-4: I doubt that there are so few studies in which temperature is used as a natural tracer under upwelling conditions (*Conant*, 2004; *Schmidt et al.*, 2006, 2007).
5. page 4306, line 9: add "mean" before "temperature gradient"
6. page 4306, line 15: An estimation within one order of magnitude is not good at all.
7. page 4306, lines 17-18: I don't think that that statement that one should consider the physical processes to be measured before designing a measurement set-up belongs into the abstract of any scientific paper. This is self speaking for any scientist.
8. page 4306, line 21: "using" rather than "both"

9. page 4307, line 21: "small inverse gradients", what do the authors mean? Small absolute values of the gradient (small $\partial |T| / \partial z$), which would make sense to me, or large gradients (small $\partial z / \partial T$)? The same phrase appears later on again, and remains confusing.
10. page 4307, line 22: Whether groundwater temperatures are higher or lower than stream temperatures is absolutely irrelevant for the analysis. The question at hand is whether there is a mean gradient at all, positive or negative.
11. page 4307, line 23: replace "less" by "smaller"
12. page 4307, line 26: add "uniform" before "vertical infiltration velocity"
13. page 4308, line 1: "no mean temperature gradient" rather then just "temperature gradient
14. page 4308, line 4: "larger" rather than "greater"
15. page 4308, line 7: Again, whether mean conduction is upwards or downwards is absolutely irrelevant.
16. Sections 2.2 & 2.3: I highly recommend presenting the combined solution right away. Also flipping the sign of v_z does not contribute to clarity. There is no need to stick exactly to the nomenclature of the cited articles.
17. page 4310, line 4: I have no idea what "anisothermal flow" means. Do you mean "temperature independent flow"?
18. page 4310, line 10: Another unclear small inverse gradient
19. page 4310, line 18: "When dispersivity is neglected": Sorry, the quoted analytical solution does not neglect dispersion/conduction at all.

20. page 4310, following Eq. (4): K_e and v_f should be introduced earlier on, where the convection-conduction equation is discussed for the first time.

21. page 4311, lines 4-8: The authors did not understand that the steady-state contribution and the sinusoidal contribution are additive. This results from the underlying *pde* to be linear and the orthogonality of different frequencies in Fourier analysis.

22. Section 2.4: I don't understand the purpose of the virtual test case at all. Steady state is steady state, and time periodic is time periodic. You must not confuse those two. This is so obvious that there is no need to perform a numerical test.

23. Page 4314, lines 17-18: This statement is utterly wrong. Eq. (3) does not depend on the sign of the temperature gradient. It depends on steady-state flow and uniform coefficients.

24. Section 3.2.1: You got me lost here at some point. Please make first clear what you are doing. Obviously, a time-varying heat-flux boundary condition is fitted to the data. However, there are head measurements in the stream and at depth. Thus, rather than relying on those heads, which should determine the volumetric flux, the specific discharge is tweeked in such a way that some temperature breakthrough curves fit. That implies inconsistencies with the head measurements. I am not convinced that this "calibrated" model is the right reference.

25. Section 3.2.2: Taking the solution relying on steady-state flow worked OK when considering some data tripples, but not with all of them. Again, this is inconsistent. The analytical solution is for the entire profile and should thus be fitted to all data points. If that leads to bad results, the expression is not valid. However, you could still work with the combined steady-state/sinusoidal expression (and maybe fit K_e while you are calibrating the model).

Let's assume that the good agreement with the steady-state solution is real: Does this imply quasi steady-state behavior? If the time scales of heat transfer are smaller than the time scales of the velocity fluctuations, the latter would not be particularly surprising.

26. Section 3.2.3: I don't quite see why the authors restrict themselves to analyzing the amplitude dampening of the dirunal signal. The phase shift does provide additional information, and of course one can use the combination of the steady-state and diurnal contributions. The statement on page 4317, line 13-15, that the majority of studies based on analyzing the periodic signal makes use of the amplitude only may be doubted. We have always taken the time shift as primary measurement, because it is the most intuitive quantity (*Vogt et al.*, 2010a,b, 2012). However, if possible, one should always take both the amplitude and dampening.

27. Page 4320, line 7. I don't quite see why a sensitivity analysis should be outside the scope of the current study. The authors could easily drop the virtual test case.

Appendix: Derivation of the Presented Analytical Expressions

Starting point of the derivation is Eq. (1). To simplify matters even more, we consider the deviation from T_∞:

$$T' = T - T_\infty \tag{7}$$

leading to:

$$\frac{\partial T'}{\partial t} + v_f \frac{\partial T'}{\partial z} - K_e \frac{\partial^2 T'}{\partial z^2} = 0 \tag{8}$$

$$
\begin{aligned}
T'(0,t) &= T_{avg} - T_\infty + A\cos\left(\tfrac{2\pi t}{P}\right) && (9)\\
\lim_{z\to\infty} T'(z,t) &= T'_\infty \forall t && (10)
\end{aligned}
$$

Fourier transformation of Eq. (8) in time yields:

$$
2\pi i f \tilde{T}' + v_f \frac{d\tilde{T}'}{dz} - K_e \frac{d^2\tilde{T}'}{dz^2} = 0\ \forall f \tag{11}
$$

subject to:

$$
\begin{aligned}
\tilde{T}'(0,f) &= (T_{avg} - T_\infty)\,\delta(f) + \tfrac{A}{2}\delta(f \pm 1P) && (12)\\
\lim_{z\to\infty} \tilde{T}'(z,f) &= 0 && (13)
\end{aligned}
$$

in which f is the ordinary frequency, $\tilde{T}'(z,f)$ is the Fourier-transform of $T'(z,t)$, i is the imaginary number, and $\delta(\cdot)$ is the Dirac delta function. The beauty of Fourier transformation is that - for linear problems with time-invariant coefficients - a time-dependent problem is replaced by a sum over all frequencies, including $f = 0$, the steady-state problem.

The general ansatz, to be solved for each frequency independently, is:

$$
\tilde{T}'(z,f) = a_1(f)\exp(\alpha_1(f)z) + a_2(f)\exp(\alpha_2(f)z) \tag{14}
$$

Substitution of Eq. (14) into Eq. (11) and rearrangement yields:

$$
\left(2\pi i f + v_e\alpha_{1,2} - K_e\alpha_{1,2}^2\right)(a_1\exp(\alpha_1 z) + a_2\exp(\alpha_2 z)) = 0 \tag{15}
$$

which holds for all values of z only if the left bracket term equals zero. Thus, α_1 and α_2 must be:

$$
\alpha_1 = \frac{v_f + \sqrt{v_f^2 + 8\pi i f K_e}}{2K_e};\ \alpha_2 = \frac{v_f - \sqrt{v_f^2 + 8\pi i f K_e}}{2K_e} \tag{16}
$$

involving square-roots of complex numbers that can be separated into real and imaginary components by:

$$
\sqrt{Re + iIm} = \sqrt{\sqrt{Re^2 + Im^2} + Re}^{\,2} + i\sqrt{\sqrt{Re^2 + Im^2} - Re}^{\,2} \tag{17}
$$

Now the coefficients in the exponentials are:

$$
\begin{aligned}
\alpha_1(f) &= Re_1(f) + iIm_1(f) && (18)\\
Re_1(f) &= \frac{v_f + \sqrt{\sqrt{v_f^4 + 64\pi^2 f^2 K_e^2} + v_f^2 2}}{2K_e} && (19)\\
Im_1(f) &= \frac{\sqrt{\sqrt{v_f^4 + 64\pi^2 f^2 K_e^2} - v_f^2 2}}{2K_e} && (20)\\
\alpha_2(f) &= Re_2(f) + iIm_2(f) && (21)\\
Re_2(f) &= \frac{v_f - \sqrt{\sqrt{v_f^4 + 64\pi^2 f^2 K_e^2} + v_f^2 2}}{2K_e} && (22)\\
Im_2(f) &= \frac{-\sqrt{\sqrt{v_f^4 + 64\pi^2 f^2 K_e^2} - v_f^2 2}}{2K_e} && (23)
\end{aligned}
$$

No matter what the sign of v_f, the real component of α_1 will always be positive, implying infinite growth of $\exp(\alpha_1 z)$ at the limit of $z \to \infty$. Hence, a_1 must be zero. (If a boundary condition at depth L is chosen, this is not necessarily the case). By contrast, the real component of α_2 is always negative, implying $\lim_{z\to\infty}\exp(\alpha_2 z) = 0$, which is consistent with the auxiliary condition.

Also, the boundary condition at $z = 0$ must be met, leading to the analytical solution in the Fourier domain:

$$\tilde{T}'(z,f) = \exp\left(\frac{v_f z}{2K_e} - \frac{\sqrt{\sqrt{v_f^4 + 64\pi^2 f^2 K_e^2} + v_f^2 2}}{2K_e} z\right) \times$$
$$\times \exp\left(-i\frac{\sqrt{\sqrt{v_f^4 + 64\pi^2 f^2 K_e^2} - v_f^2 2}}{2K_e} z\right)\left((T_{avg} - T_\infty)\,\delta(f) + \frac{A}{2}\delta(f \pm 1P)\right) \quad (24)$$

Back-transformation into the time domain, finally gives:

$$T(z,t) = T_\infty + \int_{-\infty}^{+\infty} \tilde{T}'(z,f)\exp(2\pi i f t)df \quad (25)$$
$$= T_\infty + (T_{avg} - T_\infty)\exp\left(\frac{(v_f - |v_f|)z}{2K_e}\right)$$
$$+A\exp\left(\frac{v_f z}{2K_e} - \frac{\sqrt{\sqrt{v_f^4 + \frac{64\pi^2 K_e^2}{P^2}} + v_f^2 2}}{2K_e} z\right)\cos\left(\frac{2\pi t}{P} - \frac{\sqrt{\sqrt{v_f^4 + \frac{64\pi^2 K_e^2}{P^2}} - v_f^2 2}}{2K_e} z\right) 6 \quad (26)$$

References

Conant, B. (2004), Delineating and quantifying ground water discharge zones using streambed temperatures, *Ground Water*, *42*(2), 243–257, doi:10.1111/j.1745-6584.2004.tb02671.x.

Schmidt, C., M. Bayer-Raich, and M. Schirmer (2006), Characterization of spatial heterogeneity of groundwater-stream water interactions using multiple depth streambed temperature measurements at the reach scale, *Hydrol. Earth Sys. Sci.*, *10*(6), 849–859.

Schmidt, C., B. Conant, Jr., M. Bayer-Raich, and M. Schirmer (2007), Evaluation and field-scale application of an analytical method to quantify groundwater discharge using mapped streambed temperatures, *J. Hydrol.*, *347*(3-4), 292–307, doi:10.1016/j.jhydrol.2007.08.022.

Vogt, T., P. Schneider, L. Hahn-Woernle, and O. A. Cirpka (2010a), Estimation of seepage rates in a losing stream by means of fiber-optic high-resolution vertical temperature profiling, *J. Hydrol.*, *380*(1-2), 154–164, doi:10.1016/j.jhydrol.2009.10.033.

Vogt, T., E. Hoehn, P. Schneider, A. Freund, M. Schirmer, and O. A. Cirpka (2010b), Fluctuations of electrical conductivity as a natural tracer for bank filtration in a losing stream, *Advances Water Resour.*, *33*(11, SI), 1296–1308, doi:10.1016/j.advwatres.2010.02.007.

Vogt, T., M. Schirmer, and O. A. Cirpka (2012), Investigating riparian groundwater flow close to a losing river using diurnal temperature oscillations at high vertical resolution, *Hydrol. Earth Sys. Sci.*, *16*(2), 473–487, doi:10.5194/hess-16-473-2012.

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