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Coupling diffusion and maximum entropy models to estimate thermal inertia

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A B S T R A C T

Thermal inertia is a physical property of soil at the land surface related to water content. We developed a method for estimating soil thermal inertia using two daily measurements of surface temperature, to capture the diurnal range, and diurnal time series of net radiation and specific humidity. The method solves for soil thermal inertia assuming homogeneous 1-D diffusion of heat near the land surface. The solution uses a boundary condition taken as the maximum likelihood estimate of ground heat flux made by a probabilistic uncertainty model of the partitioning of net radiation based on the theory of maximum entropy production (MEP model). We showed that by coupling the 1-D diffusion and MEP models of energy transfer at the land surface, the number of free parameters in the MEP model can be reduced from two (P — soil thermal inertia and I — thermal inertia of convective heat transfer to the atmosphere) to one (P is defined by I). A sensitivity analysis suggested that, for the purpose of estimating thermal inertia, the coupled model should be parameterized by the ratio P/I. The coupled model was demonstrated at two semi-arid sites in the southwest United States to estimate thermal inertia and these thermal inertia values were used to estimate soil moisture. We found 1) parameterizing the MEP model with a constant annual P/I value resulted in surface flux estimates which were similar to those made when daily P and I parameters were derived directly from measurements of ground heat flux (Nash-Sutcliffe efficiency > 0.95); 2) estimates of P made using the coupled model were superior to those made using the diffusion model with a common linear approximation of the ground heat flux boundary condition; and 3) thermal inertia was a better predictor of soil moisture in moderately wet conditions than in dry conditions due to a lack of sensitivity of thermal inertia to changes in soil moisture at low moisture contents.

1. Introduction

Thermal inertia, P [$Jm^{-2}\,s^{-1/2}\,K^{-1}$], is a physical property of the land surface which determines resistance to temperature change under seasonal or diurnal heating. It is a function of volumetric heat capacity, c [$Jm^{-3}\,K^{-1}$], and thermal conductivity, k [$Wm^{-1}\,K^{-1}$] of the soil or other geologic material near the surface:

$$P = \sqrt{ck}. \quad (1)$$

Thermal inertia of soil varies with moisture content due the difference between thermal properties of water ($c_w \approx 4.18$, $k_w \approx 0.59$) and air (dry: $c_a \approx 0.0013$, $k_a \approx 0.25$). The temperature of a wet soil varies less with diurnal heating than the temperature of a dry soil and a number of studies have demonstrated that it is feasible to estimate soil moisture given thermal inertia (e.g. Lu et al., 2009; Price, 1980).

The problem of estimating thermal inertia using measurements of surface temperature, perhaps in conjunction with other observations, has also been widely studied; van de Griend et al. (1985) gave a concise contemporary review and Cracknell and Xue (1996a) summarized further developments. The common approach for estimating thermal inertia is to model the Earth's surface as a 1-dimensional homogeneous diffusive half-space and derive surface temperature as a function of the ground heat flux (G) boundary condition and soil thermal properties. Cracknell and Xue (1996b) describe a classical Fourier solution to the 1-D diffusion equation which can be used to estimate a daily value of thermal inertia from two observations of surface temperature and a time series of ground heat flux measurements. The primary issue in applying this technique is that it is difficult to obtain continuous measurements of G, and a number of studies have tried to accommodate for this. For instance, Verhoef (2004) used the nighttime drop in surface temperature and an assumption that during the night, ground heat flux is equal to net radiation, and found that this led to reasonable estimates of P on clear, windstill nights. Wang et al. (2010) approximated a diffusion solution using the diurnal amplitude of ground heat flux in a way which required only two daily measurements of G. Xue and Cracknell (1995) derived a solution for P by approximating the ground heat flux boundary condition as a linear

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function of surface temperature according to Watson (1975). This required a time series of surface-incident radiation and an estimate of the phase shift between one of the harmonic functions of surface radiation and the same harmonic of surface temperature. When there were no clouds and surface radiation could be approximated as a sine curve, this was estimated as the time difference between maximum temperature and maximum radiation and only two measurements of surface temperature were necessary to derive a daily P value. When there are clouds, time series of both surface radiation and surface temperature are needed to estimate this phase shift.

Recently, Wang and Bras (2011) developed a method for partitioning net radiation into sensible, ground and latent heat fluxes based on the principle of maximum entropy production (Dewar, 2005). This method (referred to as MEP) requires two parameters: thermal inertia of the soil and a thermal inertia-like parameter representing resistance of the atmosphere to turbulent heat convection. It was derived as a probabilistic minimization of epistemic uncertainty and differs conceptually from the physically-based diffusion approach to linking ground heat flux and soil thermal inertia.

In this paper, we combine the diffusion and MEP models for the purpose of estimating daily values of soil thermal inertia. The result is a reduction in the number of parameters required for MEP partitioning of surface fluxes from two to one. The model requires only a single (daily) parameter and inputs in the form of a net radiation time series and two daily measurements of surface temperature. We show that this coupling results in an approximation of a diffusion-like representation of near-surface turbulent convection, and we chose an appropriate parameterization of the coupled model for the purpose of estimating P based on a sensitivity analysis. The ability of the model to estimate soil thermal inertia was demonstrated using measurements taken at a field site in southern Arizona, USA, and an example of estimating soil moisture from thermal inertia is provided. Finally, we provide a demonstration of the method for estimating thermal inertia using level 3 MODIS imagery taken by the Aqua platform in 2004.

2. Model development

2.1. The diffusion model

Heat flow in a one dimensional half-space with constant physical parameters, is given in terms of thermal inertia as

$$P^2 \frac{\delta T(x,t)}{\delta t} = k^2 \frac{\delta^2 T(x,t)}{\delta x^2}; \tag{2}$$

T(x,t) is temperature at depth x and time t. Boundary conditions used by Jaeger (1953) and others are

$$\left| \lim_{x\to\infty} T(x,t) \right| < \infty \tag{2.1}$$

$$T(x,0) = T_0 \tag{2.2}$$

$$-k\frac{\delta T(x,t)}{\delta x}|_{x=0} = G(t). \tag{2.3}$$

The general Fourier series solution to [2] with the properties that T is periodic in time and exponentially decaying with depth is (Carslaw & Jaeger, 1959, p65)

$$T(x,t) = T(x,0) + \sum_{n=1}^{\infty} A_n e^{-\frac{P}{k}x\sqrt{\omega n}} \cos\left(\omega nt - \frac{P}{k}x\sqrt{\omega n} - \epsilon_n\right), \tag{3}$$

ω is the fundamental frequency, ϵ_n is the phase shift of the nth harmonic of surface temperature with respect to zero time (taken here as solar noon), and A_n is the amplitude of the nth harmonic. Surface temperature is

$$T(0,t) = T(0,0) + \sum_{n=1}^{\infty} A_n \cos(\omega nt - \epsilon_n), \tag{3.1}$$

and periodic heating at the surface expressed as harmonic functions of ω is

$$G(t) = P\sum_{n=0}^{\infty} \sqrt{\omega n} A_n \cos\left(\omega nt - \epsilon_n + \frac{\pi}{4}\right) = \sum_{n=0}^{\infty} C_n \cos(\omega nt - r_n). \tag{4}$$

If G(t) are known then the magnitude ($C_n = PA_n\sqrt{\omega n}$) and phase ($r_n = \epsilon_n - \frac{\pi}{4}$) quantities can be estimated using standard discrete Fourier methods on G so that P may be derived as the ratio of measured to modeled change in surface temperature between times t_1 and t_2 (Cracknell & Xue, 1996b)

$$P = \frac{\sum_{n=1}^{\infty} \frac{C_n}{\sqrt{\omega n}} \cos\left(\omega n t_1 - r_n - \frac{\pi}{4}\right) - \sum_{n=1}^{\infty} \frac{C_n}{\sqrt{\omega n}} \cos\left(\omega n t_2 - r_n - \frac{\pi}{4}\right)}{T_{measured}(0,t_1) - T_{measured}(0,t_2)}. \tag{5}$$

Temperature *changes* are used to account for the unknown initial condition, T(0,0), and a fundamental frequency of $\omega = 1$ [day^{-1}], which describes diurnal heating, leads to a daily effective value of P from [5].

2.2. The MEP model

Given limited knowledge about any system, the most likely state of the system is the one which maximizes the statistical entropy (see Shannon, 1948) of the uncertainty probability distribution (Jaynes & Bretthorst, 2003, pp 353). Wang and Bras (2011) showed that under this consideration, the maximally likely state of the land surface energy balance is the one which minimizes the dissipation function

$$D = 2\left(\frac{G^2}{P} + \frac{H^2}{I_h} + \frac{E^2}{I_e}\right), \tag{6}$$

under the constraint

$$R = G + H + E \tag{7}$$

where R, H and E [Wm^{-2}] are net radiation, sensible heat flux and latent heat flux respectively, and I_h and I_e [$Jm^{-2}\,s^{-1/2}\,K^{-1}$] are the thermal inertia parameters related to sensible and latent heat fluxes. Wang and Bras (2009) pointed out that sensible heat flux is actually due largely to convection rather than conduction and that I_h should be interpreted as a thermal inertia-like parameter of turbulent heat transfer. Using Monin-Obukhov similarity theory (Arya, 2001), they derived I_h as

$$I_h(t) = \rho c_p \sqrt{C_1 \kappa z}\left(C_2 \frac{\kappa z g}{\rho c_p T_{ref}}\right)^{\frac{1}{6}} |H(t)|^{\frac{1}{6}} = (I)|H(t)|^{\frac{1}{6}}, \tag{8}$$

where ρ is the density of air, c_p is the specific heat capacity of air, κ is the von Karman constant, g is gravity, and C_1 and C_2 are parameters depending on the stability of the atmosphere in the surface layer with values given by Businger et al. (1971), and listed in Wang and Bras (2009); T_{ref} is a reference temperature and z is distance from the surface. We did not use these values and instead treated I, as defined by [8], and which is a daily constant parameter of the