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# Combining remotely sensed data using aggregation algorithms

W. James Shuttleworth

Department of Hydrology and Water Resources, The University of Arizona, Tucson, AZ 85721

## Abstract

This paper describes a strategic approach for providing documentation of the surface energy exchange for heterogeneous land surfaces via the simultaneous, four-dimensional assimilation of several streams of remotely sensed data into a coupled land surface-atmosphere model. The basic concepts and underlying theory behind this proposed approach are presented with the intent that this will guide, facilitate, and stimulate future research focused on its practical implementation when appropriate data from the Earth Observing System (EOS) become available. The theoretical concepts that underlie the approach are derived from relationships between the values of parameters which control surface exchanges at pixel (or patch) scale and the area-average value of equivalent parameters applicable at larger, grid scale. A three-step implementation method is proposed which involves (a) estimating grid-average surface radiation fluxes from appropriate remotely sensed data; (b) absorbing these radiation flux estimates into a four-dimensional data assimilation model in which grid-average values of vegetation-related parameters are calculated from pertinent remotely sensed data using the equations that link pixel and grid scales; and (c) improving the resulting estimate of the surface energy balance—again using scale-linking equations by estimating the effect of soil-moisture availability, perhaps assuming that cloud-free pixels are an unbiased subsample of all the pixels in the grid square.

## Introduction

The earth system science community stands on the brink of a new era of data availability with the advent of the Earth Observing System (EOS) (Asrar and Dozier, 1994; Asrar and Dokken, 1995; Asrar and Greenstone, 1995). There is potential to use these new data in combination with *in situ* observations and data from existing operational satellites to provide improved documentation of land-surface energy balance in (near) real time. This paper proposes a strategy for exploiting remotely sensed data to document land-surface energy exchanges through the development of theory that links the model parameters which control surface exchanges at pixel (or patch) scale with the area-average value of equivalent model parameters applicable at larger, model grid scale. The proposed method is thus relevant to land surfaces which comprise landscapes of heterogeneous vegetation cover. It is based around the concept of four-dimensional data assimilation (4DDA).

'Assimilation is the process of finding the model representation which is most consistent with observations' (Lorenc, 1995), but there are insufficient observations at any one time to determine the state of the Earth's system. Integration of observations in a forecast model enables the use of observations that are distributed in space and time to provide a representation of earth system processes. Charney *et al.* (1969) first suggested combining current and past data in an explicit dynamical model, using the model's prognostic equations to provide time continuity and dynamical coupling between the available data fields. This concept has evolved into the family of techniques known as four-dimensional data assimilation (Stauffer and Seaman, 1990). In essence, 4DDA incorporates a range of diverse data fields to update the state variables in a numerical model to provide that model with the best estimate of the current state of the natural environment, often so that it can then make more accurate predictions. In the context of this paper, the model used for data assimilation must be one in which the atmosphere and the land surface (and the processes that couple them) are simultaneously represented. Such a model is likely to result from improvement of the representation of the heterogeneous land-surface processes in a meteorological model.

One way to describe heterogeneous vegetation in meteorological models is to make calculations for separate patches of vegetation corresponding to several biomes present in each modelled grid square, and then to derive grid-average values by weighting the surface energy fluxes calculated for each patch by the fractional area of the corresponding vegetation class present in the grid square.

This is the so-called 'mosaic' approach (e.g., Koster and Suarez, 1992; Bonan, 1996). It is a conceptually simple and technically feasible way to represent the effect of surface heterogeneity in the case of predictive weather and climate models when there is no attempt to distribute meteorological variables spatially within the modelled grid area.

When used in predictive models, one of the attractive features of a mosaic model is that the soil moisture status of each patch of vegetation represented in the model is calculated separately. However, in the case of a model used to document surface energy balance via 4DDA, this feature is likely to complicate the use of mosaic models because of the nature of the data that must be assimilated to update soil moisture. One possible source of relevant data is space-borne, L-band, passive microwave sensors. The technical constraints on these satellite-borne microwave sensors are such that in the foreseeable future (and certainly in the EOS era), the data they will provide will correspond to spatial average, near-surface soil moisture over areas which are often much greater than that of the patches of vegetation in a heterogeneous landscape. Thus, it might be considered inconsistent to assimilate these data with separately-modelled patches of vegetation (with different soil moisture states) in a mosaic model. Other potential sources of information on soil moisture information, such as surface temperature (see later), are often only available for portions of the grid area used in the 4DDA model. Later in this paper it is suggested that this may not preclude their use, providing the soil moisture status deduced for the cloud-free portion of the grid square can be assumed representative of the whole grid square. Implementing this assumption is reasonably simple if aggregate parameter sets which specify a single 'representative' vegetation cover are calculated for both the cloud-covered and cloud-free portions of the grid area. However, if, as in the case of the mosaic model, several independent patches of vegetation are used, and if updating is required for each of the separately modelled soil moisture stores represented in such a model, then calculations are required for the cloud-free and cloud-covered pixels corresponding to each vegetation class represented in each model modelled grid square. The calculation may thus become cumbersome.

An alternative way to represent heterogeneous land cover involves using a single model of the grid-average surface exchanges, with the values of vegetation-related parameters chosen to represent the area average or 'aggregate' behaviour of the heterogeneous vegetation mix present in the area represented. There has been progress in specifying area-average parameters on two fronts, one being essentially empirical and the other theoretical. The empirical approach (e.g. Mason, 1988; Blyth *et al.*, 1993; Noilhan and Lacarrere, 1995; Arain *et al.*, 1996, 1997) is to postulate and then to test hypothetical rules (often called 'aggregation rules'; Shuttleworth, 1991) to give parameters applicable at larger scales by combining the parameters that control surface exchanges for small plots of uniform land cover. In the theoretical approach to defining aggregate parameters (e.g. Lhomme, 1992; McNaughton, 1994; Raupach, 1995; and Raupach and Finnigan, 1995, 1997), a model is adopted which provides reasonable descriptions of surface-atmosphere exchanges for small plots of uniform land cover, such models usually being based on the Penman-Monteith equation (Monteith, 1965). Assuming that this same model can also be used to describe the area-average behaviour of heterogeneous land cover, it is possible to derive theoretical equations that link the parameters required in the model when applied at large scale with those which apply for individual small plots.

## General approach

An aggregation algorithm is conceived as a method which seeks to make optimum, simultaneous use of several parallel streams of spatially distributed remotely sensed data which are available at a (pixel) scale that is less than the grid scale of the model used to assimilate the data. In the context of four-dimensional data assimilation (4DDA) within meteorological models, the words 'data assimilation' have come to imply the altering of modelled state variables by way of a balance between observational and model errors. However, in the context of the method proposed here, the word 'assimilation' retains its broader, original meaning, and thus data assimilation may include the direct replacement of model estimates with values based on satellite observations.

The objective is to give improved diagnosis of surface-atmosphere exchanges by developing mathematical methods which are similar to those which have been suggested for blending the values of vegetation-related parameters for a heterogeneous landscape to give equivalent area-average parameter values (e.g. McNaughton, 1994; Raupach, 1995; Raupach and Finnigan, 1995; 1997). The proposed strategy is explicitly structured around the three main factors that control land-surface energy exchange which are, in approximately descending order of importance, (a) the energy available at the Earth's surface for return to the atmosphere; (b) the nature of the land surface (e.g. the vegetation cover present); and (c) the availability of water which is accessible to the atmosphere in the soil. Different types of remotely sensed data relate to each of these controls.

In the case of the first control, i.e. available surface energy, the relevant remotely sensed data are instantaneous estimates of surface radiation fluxes made at regular (perhaps half-hourly) intervals, most likely derived using operational satellites such as those in the Geostationary Operational Environmental Satellite (GOES) series. There are several existing, well-proven algorithms available for deriving such surface radiation estimates (e.g. Pinker and Ewing, 1985; Pinker and Laszlo, 1990; 1992), and there is evidence that remotely sensed estimates of (at least solar)

surface radiation fluxes are reasonably reliable, and that they are superior to many model-calculated estimates (Pinker *et al.*, 1994). Applying algorithms that yield remotely sensed estimates of surface radiation fluxes often involves averaging over all the pixels in a model's grid square to give grid-average estimates of the surface radiation fluxes. Such averaging helps mitigate against the fact that the sampled satellite image provides only an instantaneous measure of the spatial distribution of surface radiation. Spatial averaging is thus used as a substitute for time averaging, under the assumption that there is little persistent correlation between surface features and overhead cloud cover.

One feature frequently present in surface radiation algorithms is a classification of pixels as cloud-free (as opposed to cloud-covered or partially cloud-covered), and this classification is used in the third step of the aggregation algorithm approach described later. If such a classification is not made during the calculation of remotely sensed estimates of surface radiation, it will need to be carried out as an additional process in the aggregation algorithm. The particular nature of the algorithm used to derive surface radiation fluxes is irrelevant in this paper. However, it is assumed here that grid-average values of surface radiation fluxes are indeed being derived routinely and regularly from satellite data using an appropriate algorithm, and that these data are available to be assimilated into the model used for 4DDA as an important (and arguably the primary) control on a model-calculated documentation of land surface-atmosphere energy exchange.

If water accessible by the atmosphere in the soil is plentiful, the nature of the underlying land surface provides the next most important control on land-surface energy exchange. Two categories of remotely sensed information are relevant in this case. The first category includes maps of land-cover class. The general nature of the vegetation, i.e. its classification into one of several (often model-specific) biomes is important because vegetation class influences important, plant morphology-dependent and physiology-dependent parameters. In addition, remotely sensed data may provide an indirect measure of seasonal variations in the amount of green vegetation present for each land-cover class.

The character of the relevant remotely sensed information used to specify vegetation cover class and the extent of leaf cover is fundamentally different to that for surface radiation. Land-cover parameters change more slowly with time, which is fortunate because the relevant remotely sensed information is usually only intermittently available because of cloud cover. There are several methods already available for classifying the general nature (or biome) of land cover (e.g. Eidenshink and Faundeen, 1994; Running *et al.*, 1994), and also methods for determining season changes in the amount of green vegetation present in each pixel (e.g. Reed *et al.*, 1994; Sellers *et al.*, 1996b). Improved classification methods and algorithms will no doubt appear in due course, but the details of these are again independent of the present paper.

Using the procedures outlined above, it is reasonable to propose the use of a coupled land surface-atmosphere model to provide a grid-average diagnosis of surface energy exchanges by assimilating remotely sensed estimates of grid-average surface radiation fluxes, while at the same time making use of remotely sensed information on land-cover class and green vegetation cover. To go further, and to assimilate remotely sensed information relevant to the third control—soil moisture availability—is more complex. In this case, the remotely sensed information will often be indirect (e.g. radiometric surface temperature) or incomplete (e.g. near-surface soil moisture only). To compound the problem, because of cloud cover, indirect measures of soil-moisture availability might be intermittently available or might be available only for portions of the grid square. Thus, when diagnosing surface energy balance, the details of an aggregation algorithm will vary depending on the nature and assumed reliability of the remotely sensed data used to estimate the grid-average soil-moisture availability.

This paper seeks to provide the underlying concepts and basic theory behind the aggregation algorithm approach. To do this, remotely sensed surface temperature is selected as an example diagnostic of soil-moisture availability. If the surface radiation and the nature and behaviour of the vegetation and soil are correctly described, soil moisture availability becomes the primary control on the difference between the surface temperature and that of the overlying air. Alternative diagnostic variables of soil moisture are potentially available, and these might well ultimately prove superior—near-surface soil moisture derived from microwave sensors is an obvious example. It is anticipated that the aggregation algorithm method which is proposed here in rudimentary form will evolve and improve through the use of alternative or supplementary measures of grid-average soil-moisture availability. Ultimately, several different measures of moisture availability might be used, with appropriate weighting applied in the 4DDA process between these alternatives according to their reliability.

In fact, selecting the example of remotely sensed surface temperature in the present paper is instructive because it allows discussion of methods required when data relevant to soil moisture are available for only some of the pixels in a grid square. In this case, it is necessary to assume that there is no persistent correlation between the location of clouds and the location of available soil water in the grid square. In other words, it is necessary to assume that, on average, the visible portion of the grid (if any is visible at all) corresponds to an area which is representative of the grid-average available soil moisture. Clearly, there may be problems with this assumption if the grid size of the model is large enough to allow within-grid correlation between precipitation and (say) topography or earlier precipitation.

Nonetheless, making this assumption, and using remotely sensed information for surface radiation and for

vegetation class and leaf cover for the cloud-free portion of the grid, it is possible to estimate the area-average surface energy balance for the cloud-free portion. Comparing this with the surface energy balance derived using remotely sensed surface temperature (rather than modelled surface temperature) should allow the correction of the modelled soil moisture for the cloud-free portion (e.g. Toth *et al.*, 1998). Assuming that, on average, the cloud-free pixels are a reasonable subsample of all the pixels in the grid square, the modified available soil moisture can then be applied to the grid as a whole, and arguably the modelled grid-average surface energy balance so improved.

Thus, in summary, the aggregation algorithm approach to documenting surface energy balance using remotely sensed data involves three steps, as follows:

(a) The first step is to make estimates of grid-average surface radiation fluxes from appropriate remotely sensed data and, if not already part of the algorithm used to estimate radiation, to identify pixels in the grid square which are totally cloud-free.
(b) The second step is to absorb these radiation estimates into a four-dimensional data assimilation model in which the area-average vegetation parameters applicable at grid scale are calculated at each model time step from remotely sensed data using linking equations between grid scale and pixel scale parameters. Running the 4DDA model will provide a source of transient, model-calculated, area-average atmospheric variables and soil moisture for each grid square, and an estimate of grid-average surface energy fluxes which acknowledges the presence of heterogeneous vegetation and which responds to the remotely sensed surface radiation fluxes.
(c) The third step is to estimate the surface energy fluxes for the cloud-free portion of each grid square, perhaps using some indirect, remote-sensing measure; in this paper, surface temperature is used as an example. Comparison between these estimated surface fluxes with the calculated surface energy balance for the same cloud-free area in the 4DDA model allows an estimate of available soil moisture in the cloud-free area. It is then assumed that nudging the grid-average soil moisture towards the estimated soil moisture for the cloud-free portion will improve the 4DDA model's ability to document grid-average surface energy exchange by modifying the surface energy partition.

Use of an aggregation algorithm approach should allow a diagnosis of the grid-average surface latent and sensible heat fluxes which makes best simultaneous use of several streams of pixel-scale remote-sensing data. This likely also contributes towards improved diagnosis of the grid-average near-surface weather variables.

## Aggregation theory

Two requirements are often applied to define relationships that combine vegetation-related parameters relevant at pixel scale to give a description of area-average surface fluxes. The first is fundamental, namely that the area-average scalar fluxes must be the same at the two scales. The second is that it is convenient if the 'model' used to describe area-average land-surface-atmosphere exchanges at grid scale has the same form as the 'model' used to describe such land-surface-atmosphere exchanges at pixel scale (McNaughton, 1994). In principle, these requirements might be used to provide linking equations for the parameters used with a model of any complexity. However, to maximise the generality of the present analysis, here we adopt linking equations that result when these two requirements are applied to very simple (but widely used) models of surface exchanges. In the case of momentum exchange, the 'model' used is to assume that mixing length theory applies in the surface layer, with wind speed following a logarithmic profile. In the case of energy fluxes, the 'model' adopted is the Penman-Monteith equation (Monteith, 1965). In practice, the majority of physically realistic land surface-atmosphere models are based on these two simple models, albeit they may be applied implicitly and with seemingly greater complexity.

In the case of momentum exchange, applying the above requirements yields the result:

$$\frac{1}{R_{a,M}} = \left[\sum_{i}^{N} \frac{w_i}{r_{a,M,i}}\right] \qquad (1)$$

where $R_{a,M}$ and $r_{a,M,i}$ are the grid-average and pixel-average aerodynamic resistances, respectively, $w_i$ is the fractional area of pixel $i$ in the grid square, and $N$ is the total number of pixels in the grid square. For convenience, the symbols used in this and subsequent equations are listed in Appendix 1. This equation, when applied in neutral conditions, has been used to define the grid-average aerodynamic roughness length in terms of the aerodynamic roughness length applicable to individual pixels (Wieringa, 1986; Mason, 1988; Shuttleworth, 1991; Arain *et al.*, 1996, 1997).

In the case of surface energy fluxes, the albedo of the surface is an important parameter at both pixel scale and grid scale. Assuming the surface energy balance is described by the Penman-Monteith equation, so are the (vegetation-related) aerodynamic resistance and the surface resistance and, if considered appropriate, the radiative resistance used in that equation. The analysis of Raupach (1995) is adopted here for his 'simple case', i.e. when the aerodynamic resistances between the canopy and the overlying atmosphere for latent and sensible heat are assumed equal and when the longwave radiative coupling between canopy level and the near-surface atmosphere is deemed negligible. With these simplifications, the Penman-Monteith equation applied at grid scale and pixel scale has the form:

$$E = \frac{\Delta R_a A + \rho\lambda D}{\Delta R_a + (R_a + R_s)} \quad (2)$$

and

$$E_i = \frac{\Delta r_{a,i} A_i + \rho\lambda D}{\Delta r_{a,i} + (r_{a,i} + r_{s,i})} \quad (3)$$

respectively, where $E$ and $E_i$ are the grid-average and pixel-average latent heat fluxes, respectively; $A$ and $A_i$ are the grid-average and pixel-average available energy, respectively; $R_a$ and $r_{a,i}$ are the aerodynamic resistances for energy fluxes at grid scale and pixel scale, respectively; $R_s$ and $r_{s,i}$ are the surface resistances applicable at grid scale and pixel scale, respectively; $\rho$ is air density; $\lambda$ is the latent heat of vaporisation of water; $D$ [$= q_{sat}(\theta) - q$] is the potential saturation deficit of the ambient air at a specified level, with $\theta$ the potential temperature and $q$ specific humidity at that height; and $\Delta$ [$= (\lambda/c_p)\, dq_{sat}/dT$] is the dimensionless slope of the saturation specific humidity $q_{sat}(T)$ as a function of temperature $T$, where $c_p$ is the isobaric specific heat of air. The surface energy balance (already implicit in Eqns. 1 and 2) gives the sensible heat fluxes at grid scale, $H$, and pixel scale, $H_i$, thus:

$$H = A - E \quad (4)$$

$$H_i = A_i - E_i \quad (5)$$

By applying McNaughton's (1994) requirements for linking between scales to Eqns. 2 and 3, Raupach (1995) derived the relationships:

$$R_a = \frac{R_d}{A} \sum_i^N \frac{w_i A_i r_{a,i}}{r_{a,i}(\Delta + 1) + r_{s,i}} \quad (6)$$

and:

$$R_s = \frac{R_d}{A} \sum_i^N \frac{w_i A_i r_{s,i}}{r_{a,i}(\Delta + 1) + r_{s,i}} \quad (7)$$

where:

$$R_d = \left[ \sum_i^N \frac{w_i}{r_{a,i}(\Delta + 1) + r_{s,i}} \right]^{-1} \quad (8)$$

Equations 1, 6, 7 and 8 are the basic equations that link aerodynamic and surface resistance between pixel scale and grid scale and provide the basis for the analysis given in this paper.

## Implementing an Aggregation Algorithm

In the following, the theory which underlies essential aspects of the application of an aggregation algorithm is described, taking as an example the case when available soil moisture is indirectly estimated from remotely sensed surface temperature.

### SURFACE RADIATION FLUXES

Many surface radiation algorithms can only reliably estimate $S$, the grid-average downwelling surface radiation in the solar wave band. For simplicity, it is convenient to neglect any dependence of albedo on the zenith angle of incident radiation. Thus, assuming that, at each time step the 4DDA model calculates $A_m$, the grid-average surface energy available at the land surface (i.e. the so-called available energy), and that in so doing it also calculates $S_{n,m}$, the grid-average net solar radiation. It may be possible to calculate an improved estimate of $A$, the grid-average available energy, by replacing the model-calculated net solar radiation by the remotely sensed estimate of net solar radiation for the observed (as opposed to modelled) cloud cover, thus:

$$A = A_m - S_{n,m} + S \sum_i^N w_i (1 - \alpha_i) \quad (9)$$

where $N$ is the number of pixels in the grid square; and $\alpha_i$ is the albedo for pixel $i$, this being ascribed via a look-up table from the remotely sensed land-cover class for that pixel.

Some remote-sensing algorithms may attempt to estimate longwave radiation. If, for instance, an estimate of, $L_n$, the grid-average net longwave radiation, is available, and if this estimate is deemed reliable, then an improved estimate of grid-average available energy would be given by additionally replacing the model-calculated net longwave radiation by the remotely sensed estimate of net longwave radiation, thus:

$$A = A_m - S_{n,m} + S \sum_i^N w_i (1 - \alpha_i) - L_{n,m} + L_n \quad (10)$$

where $L_{n,m}$ is the grid-average net longwave radiation exchange at the surface calculated in the 4DDA model.

### AREA-AVERAGE COVER-RELATED PARAMETERS

The following analysis closely parallels that in Shuttleworth *et al.* (1997) and is therefore most easily understood after reading that paper.

#### *Aerodynamic Resistance*

Given a pixel-scale land-cover classification, the values of aerodynamic roughness length and zero plane displacement can be considered available at pixel scale via a (usually model-specific) look-up table. By analogy with the procedure used to evaluate the grid-average aerodynamic roughness (Wieringa, 1986; Mason, 1988; Shuttleworth *et al.*, 1997), in neutral conditions:

$$r_{a,M,i} = (\kappa^2 U_b)^{-1} \ln^2 \left( \frac{(z_b - d_i)}{z_{0,i}} \right) \quad (11)$$

where $\kappa$ is the von Karman constant, and $U_b$ is the grid-average wind speed predicted at a 'blending height', $z_b$, by

the 4DDA model. For a discussion of blending height, see Wieringa (1986), Mason (1988) and Arain *et al.* (1996)—often it is assumed to be the lowest modelled level. With a prescribed value of $U_b$, Eqn. 1 might be used with Eqn. 11 to calculate $R_{a,M}$ (e.g. Mason; 1988). In practice, this is equivalent to applying the two rules:

$$d = \sum_i^N w_i d_i \tag{12}$$

$$\ln^{-2}\left(\frac{(z_b - d)}{z_0}\right) = \sum_i^N w_i \ln^{-2}\left(\frac{(z_b - d_i)}{z_{0,i}}\right) \tag{13}$$

where $d$ is the grid-average value of zero plane displacement, and $z_o$ is the grid-average aerodynamic roughness length.

All land-surface-atmosphere models make assumptions regarding the relationship between the aerodynamic roughness relevant for momentum transfer and that relevant for energy flux transfer. At grid scale, this relationship is written in the generic form as the function F in the equation:

$$R_a = F(R_{a,M}) \tag{14}$$

where $R_a$ is the required value of aerodynamic resistance for energy transfer, and $R_{a,M}$ is the aerodynamic resistance for momentum transfer applicable at grid scale. This relationship will often involve the grid-average values of zero plane displacement, $d$, and the grid-average aerodynamic roughness length, $z_o$, derived from Eqns. 12 and 13 when making the grid-scale calculations of the aerodynamic resistance applicable for latent and sensible heat fluxes.

*Surface Resistance*

In the following, it is assumed that, for each pixel in the grid, the radiation fluxes are equal to the grid-average values derived from the radiation flux algorithm. In principle, the remotely sensed image contains information on the spatial distribution of radiation, but this is an instantaneous distribution. As mentioned earlier, radiation algorithms often assume that spatial averaging provides a surrogate for time averaging, so that taking a spatial average across the grid square partly compensates for the fact that the remotely sensed image is instantaneous. Here, it is necessary to assume uniform radiation fluxes across the 4DDA model grid in order to be consistent with this strategy. Thus, the grid-average available energy, $A$, is assumed to apply uniformly across the model grid, and weighting by $A_i$ in Eqns. 7 and 8 is irrelevant. Removing such weighting gives the simpler equations:

$$R_a = R_d \sum_i^N \frac{w_i r_{a,i}}{r_{a,i}(\Delta + 1) + r_{s,i}} \tag{15}$$

$$R_s = R_d \sum_i^N \frac{w_i r_{s,i}}{r_{a,i}(\Delta + 1) + r_{s,i}} \tag{16}$$

At some future time (but perhaps not within the currently defined lifetime of EOS), it is possible that operational satellites will provide data from which surface radiation fluxes can be derived with sufficient frequency to enable calculations of pixel-specific values of net solar radiation averaged over the time step of the 4DDA model. Calculation of area-average surface resistance would then merely be made using Eqn. 7 rather than Eqn. 16.

Equations 8 and 16 (or perhaps in the future Eqns. 7 and 8) can be used to give the effective, grid-average value of surface resistance, $R_s$, as long as it is possible to provide estimates of $r_{a,i}$ and $r_{s,i}$ for each pixel in the grid square. The requirement that the models used at grid scale and pixel scale have the same form (McNaughton, 1994) means that the equation used to calculate aerodynamic resistance for energy transfer applicable at pixel scale, $r_{a,i}$, must have the same form as Eqn. 14, thus:

$$r_{a,i} = F(r_{a,M,i}) \tag{17}$$

For the purposes of illustrating the aggregation algorithm approach, a generic form for the surface resistance, $r_{s,i}$, is adopted, namely:

$$r_{s,j} = r_{s,j}(S,D,T,c,M_s,L_i,V_i,C_i \ldots) \tag{18}$$

In this equation, $L_i$, $V_i$, and $C_i$ (which may be required to calculate $r_{s,j}$ in the model) are, respectively, the leaf area index, the fractional vegetation cover, and a model-specific constant for the $i$th pixel. The constant $C_i$ can be identified variously as, for example, the minimum surface resistance for the entire canopy (Dickinson *et al.*, 1986, 1993; Sellers *et al.*, 1986), the maximum photosynthetic rate (Sellers *et al.*, 1996a; 1996b), or the minimum surface resistance at the top of the canopy (Dickinson *et al.*, 1998). Here, we assume that the pixel-specific values of $C_i$ are available, these being derived from a look-up table which is indexed to the remotely sensed land-cover class for each pixel. It is also assumed that values of $L_i$ and $V_i$ can be calculated from remotely sensed data using an algorithm which has been appropriately formulated for each land-cover class represented in the 4DDA model. However, in the absence of any knowledge of pixel-specific values for $S$, the solar radiation; $D$, the vapour pressure deficit; $T$, the near-surface air temperature; $c$, the carbon dioxide concentration in the atmosphere; and $M_s$, the available soil moisture, and, indeed, any other near-surface variables that may be required in the 4DDA model, it is necessary to assume that their grid-average values apply in Eqn. 18.

Equations 8 and 16 can then be combined to give the grid-average value of $R_s$ for each model time step, thus:

$$R_s = \left[\sum_i^N \left(\frac{w_i r_{s,i}}{(\Delta + 1)r_{a,i} + r_{s,i}}\right)\right] \Big/ \left[\sum_i^N \left(\frac{w_i}{r_{a,i}(\Delta + 1) + r_{s,i}}\right)\right] \tag{19}$$

with $\Delta$ evaluated at the modelled near-surface air temperature, $r_{s,i}$ given by Eqn. 18, and $r_{a,i}$ given by Eqn. 17 with the required value of $U_b$ taken from 4DDA model.

SOIL MOISTURE ESTIMATES

The fact that such data might not be available at each time step is not necessarily a critical problem because soil moisture is a reasonably conservative state variable in the 4DDA model. Knowledge that improves the estimated value of soil moisture at one time step will propagate forward in time and, to some extent, improve subsequent estimates of surface energy exchanges. However, ultimately, of course, this improvement is lost through model drift.

Here, it is assumed that cover-specific algorithms are available that relate the remotely sensed surface temperature, $T_{s,R,i}$, to $T_{s,a,i}$, the 'aerodynamic' surface temperature which is implicit in the Penman-Monteith equation. For the land cover present in pixel $i$, such relationships are represented in generic form by the function t in the equation:

$$T_{s,a,i} = t_i(T_{s,R,i}) \tag{20}$$

From simple aerodynamic theory, the area-average sensible heat flux for the cloud-free portion of the grid square can be estimated from the equation:

$$H' = \frac{1}{W'}\sum_{i}^{N}\left\{\delta_i w_i \rho c_p \frac{T - t_i(T_{s,R,i})}{r_{a,i}}\right\} \tag{21}$$

where $\delta_i$ is a function which is unity for cloud-free pixels and zero for pixels that are partially or entirely covered by cloud, and weighting factor for cloud-free pixels, $W'$, is given by:

$$W' = \sum_{i}^{N}\delta_i w_i \tag{22}$$

The discrepancy between $H'$ and $H'_m$, the 4DDA model-calculated, area-average sensible heat flux for the clear-sky pixels in the grid square (calculated with available energy derived using solar radiation from the remote-sensing algorithm for this subset of pixels), arguably provides a measure of the error in the modelled soil moisture, $M_s$. Changing soil-moisture status will likely have the most effect on the modelled sensible heat by changing the surface energy partition, but there could also be some effect resulting from changes in the available energy associated with (soil surface temperature-dependent) modifications in upward longwave radiation and the ground heat flux. Thus, an iterative procedure is required with the improved soil-moisture estimates, $M'_s$, within each iteration made on the basis of a Taylor expansion from:

$$M'_s \approx M_s - (\partial H'_m / \partial M_s)^{-1}(H' - H'_m) \tag{23}$$

and the available energy then re-calculated from the land-surface model prior to the next iteration.

Making this (albeit model-dependent) improved estimate of soil moisture in any case requires that additional calculations are made to provide area-average variables and parameters which relate only to the clear-sky pixels present in the grid square. Thus, the available energy for cloud-free pixels, $A'_m$, is needed and it is given by an equation equivalent to Eqn. 9, that is:

$$A'_m = A_m - S_{n,m} + \frac{S'}{W'}\sum_{i=1}^{N}\delta_i w_i(1-\alpha_i) \tag{24}$$

where $S'$ is the value of downwelling solar radiation at the surface estimated in cloud-free conditions within the surface radiation algorithm. The area-average sensible flux for the cloud-free portion of the grid follows from the surface energy balance, thus:

$$H'_m = A'_m - E'_m \tag{25}$$

where $E'_m$ is the area-average latent heat flux for the cloud-free portion of the grid, which is given by an equation equivalent to Eqn. 2, that is:

$$E'_m = \frac{\Delta R'_a A'_m + \rho\lambda D}{\Delta R'_a + (R'_a + R'_s)} \tag{26}$$

In Eqn. 26, the value of the surface resistance appropriate for cloud-free pixels is given by:

$$R'_s = \left[\sum_{i}^{N}\delta_i\left(\frac{w_i r_{s,i}}{r_{a,i}(\Delta+1)+r_{s,i}}\right)\right]\Bigg/\left[\sum_{i}^{N}\delta_i\left(\frac{w_i}{r_{a,i}(\Delta+1)+r_{s,i}}\right)\right] \tag{27}$$

and the value of $R'_a$ is given by:

$$R'_s = F(R'_{a,M}) \tag{28}$$

in which $R'_{a,M}$ is the effective area-average aerodynamic resistance for momentum transfer for the cloud-free pixels which is now calculated using the zero plane displacement, $d'$, and aerodynamic roughness length, $z'_o$, derived from:

$$d' = \frac{1}{W'}\sum_{i}^{N}\delta_i w_i d_i \tag{29}$$

$$\ln^{-2}\left(\frac{(z_b - d')}{z_0}\right) = \frac{1}{W'}\sum_{i}^{N}\delta_i w_i \ln^{-2}\left(\frac{(z_b - d_i}{z_{0,i}}\right) \tag{30}$$

The value of $(\partial H'_m/\partial M_s)$ required to implement the soil-moisture correction from Eqn. 23 within each iteration cycle is estimated by applying the chain rule from:

$$\frac{\partial H'_m}{\partial M_s} = \left(\frac{\partial H'_m}{\partial R'_s}\right)\left(\frac{\partial R'_s}{\partial M_s}\right) \tag{31}$$

Combining Eqns. 25 and 26 and differentiating with respect to $R'_s$ gives:

$$\frac{\partial H'_m}{\partial R'_s} = \frac{E'_m}{R'_a(\Delta+1)+R'_s} \tag{32}$$

while differentiating Eqn. 27 with respect to $M_s$ gives:

$$\left(\frac{\partial R_s'}{\partial M_s}\right) = Y^{-2}\left[Y\left(\frac{\partial X}{\partial M_s}\right) - X\left(\frac{\partial Y}{\partial M_s}\right)\right] \quad (33)$$

with:

$$Y = \sum_i^N \delta_i \left(\frac{w_i}{r_{a,i}(\Delta+1) + r_{s,i}}\right) \quad (34)$$

$$X = \sum_i^N \delta_i \left(\frac{w_i r_{s,i}}{r_{a,i}(\Delta+1) + r_{s,i}}\right) \quad (35)$$

$$\left(\frac{\partial X}{\partial M_s}\right) = \sum_i^N \delta_i \left(\frac{w_i r_{s,i} r_{a,i}(\Delta+1)}{(r_{a,i}(\Delta+1) + r_{s,i})^2}\right)\left(\frac{\partial r_{s,i}}{\partial M_s}\right) \quad (36)$$

$$\left(\frac{\partial Y}{\partial M_s}\right) = \sum_i^N \delta_i \left(\frac{w_i r_{s,i}}{(r_{a,i}(\Delta+1) + r_{s,i})^2}\right)\left(\frac{\partial r_{s,i}}{\partial M_s}\right) \quad (37)$$

Substituting Eqns. 32 and 33 with the model-specific function $(\partial r_{s,i}/\partial M_s)$ into Eqn. 31 provides the required value of $(\partial H_m'/\partial M_s)$ to allow successive correction of the soil moisture using Eqn. 23 during the iterative cycle.

## Concluding Comments

It is clear that much research is required before the aggregation algorithm approach proposed in this paper can be implemented with confidence because the method assumes that acceptable, remotely sensed observations relevant to the surface energy balance are readily available. This is not yet the case. Thus, continued effort is required to improve and validate algorithms which estimate radiation fluxes from satellite data and, as computer resources improve, there will likely be a greater emphasis on providing estimates for smaller grid scales. Demand for radiation estimates at smaller scale will in turn generate demand for more frequent remotely sensed images because some of the benefit of spatial averaging will be lost and additional temporal sampling is needed to compensate for this. There is also a continuing need to improve the definition of land-cover classes from remotely sensed data and for research to validate the accuracy of such classification methods. The aggregation algorithm approach also motivates further research to improve and validate the relationship between green leaf area and relevant satellite data for different land-cover classes.

Understanding the difference between the radiometric surface temperature observed from satellites and the aerodynamic surface temperature implicit in the Penman-Monteith model is particularly important. Reconciling these two is critical if remotely sensed surface temperature data are to have value for documenting the surface energy balance in general and for estimating soil-moisture availability in particular. Understanding the difference between radiometric and aerodynamic surface temperature is likely to be particularly challenging in the case of sparse canopies. However, most of the issues involved are not addressed by the aggregation theory that underlies the aggregation algorithm approach because they are associated with physical processes which occur at patch scale or less. Developing the capability to estimate soil moisture directly from remotely sensed data is a high priority because of the inherent difficulties of using indirect measures of soil moisture availability. L-band sensors are known to have potentially greater capability and providing relevant algorithms and quantifying their reliability as a function of land-cover class therefore clearly merits emphasis. A space-borne, passive microwave L-band system is currently a major omission from the range of EOS sensors.

Within-grid variations in near-surface wind speed are ignored in the present paper. Such variations are possible and, indeed, likely in regions of marked topography. Their effect might be significant for models with a large grid scale because they may generate variations in the aerodynamic resistance inside the grid which influences the summations used in the aggregation algorithm. Studies with coupled surface-atmosphere models operating at mesoscale in regions with significant topography would help determine the importance or otherwise of such wind speed variations on the grid surface energy balance.

Notwithstanding the substantial challenges that evidently remain, the purpose of this paper is to provide guidance on how diverse streams of remotely sensed data available at different pixel scales can be brought together at a 4DDA model grid scale to give diagnosis of the surface energy balance. The present paper is motivated by the author's perceived need for greater organisation and structure in the strategy behind research relevant to meeting this goal, and by a desire to share this suggested strategy in a timely manner. The practical application of the proposed strategy described in this paper is the subject of ongoing research (http//:www.hwr.arizona.edu/~shuttle/aggregate.htmh). The expectation is that such investigation and additional research which is hopefully stimulated by this paper will yield a system capable of documenting surface exchanges when data from EOS become available.

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## References

Arain, M.A., Michaud, J.D., Shuttleworth, W.J. and Dolman, A.J., 1996. Testing of vegetation parameter aggregation rules applicable to the Biosphere-Atmosphere Transfer Scheme (BATS) at the FIFE site, *J. Hydrol.*, 177, 1–22.

Arain, M.A., Michaud, J.D., Shuttleworth, W.J.. Yang, Z.-L. and Dolman, A.J., 1997. Mapping surface cover parameters using aggregation rules and remotely sensed cover classes. *Quart. J. Roy. Meteorol. Soc.*, 123(B), 2325–2348.

Asrar, G. and Dozier, J., 1994, *Science Strategy for the Earth Observing System.* American Institute of Physics Press, 119 p.

Asrar, G. and Dokken, D.J., 1995. *The State of Earth Science from Space: Past Progress, Future Prospects.* American Institute of Physics Press, 159 p.

Asrar, G. and Greenstone, R., 1995. *MTPE/EOS Reference Handbook.* NASA Press NP-215, 277 p.

Blyth, E., A.J. Dolman and Wood, N., 1993. Effective resistance to sensible and latent heat in heterogeneous terrain. *Quart. J. Roy. Meteorol. Soc.*, **119**, 423–442.

Bonan, G.B., 1996. *A land surface model (LSM version 1.0) for ecological, hydrological, and atmospheric studies: technical description and user's guide.* NCAR Technical Note NCAR/TN-417+STR. National Center for Atmospheric Research, Boulder, Colorado, 150 p.

Charney, J.K., Halem, M. and Jastrow, R.R., 1969. Use of incomplete historical data to infer the present state of the atmosphere. *J. Atmos. Sci.*, **26**, 1160–1163.

Dickinson, R.E., Henderson-Sellers, A., Kennedy, P.J. and Wilson, M.F., 1986. *Biosphere-Atmosphere Transfer Scheme (BATS) for the NCAR Community Climate Model*, Technical Note NCAR/TN-275+STR, 69 p. [Available from National Center for Atmospheric Research, PO Box 3000, Boulder, Colorado.]

Dickinson, R.E., Henderson-Sellers A. and Kennedy, P.J., 1993. *Biosphere-Atmosphere Transfer scheme (BATS) Version 1e* as coupled to the NCAR Community Climate Model, Technical Note NCAR/TN-383+STR, 72 p. [Available from National Center for Atmospheric Research, PO Box 3000, Boulder, Colorado.]

Dickinson, R.E., Shaikh, M. Bryant, R. and Graumlich, L., 1998. Interactive canopies for a climate model, *J. Climate* (in press).

Eidenshink, J.C. and Faundeen, J.L., 1994. The 1 km AVHRR global land data set—first stages in implementation. *Int. J. Remote Sens.*, **15**, 3443–3462.

Koster, R.D. and Suarez, M.J., 1992. A comparative analysis of two land surface heterogeneity representations. *J. Climate*, **5**, 1379–1390.

Lhomme, J.P., 1992. Energy balance of heterogeneous terrain: averaging the controlling parameters. *Agric. For. Meteorol.*, **61**, 11–21.

Lorenc, A.C., 1995. *Atmospheric Data Assimilation.* Meteorological Office Forecasting Research Division Scientific Paper No 34. Meteorological Office, Bracknell, UK.

Mason, P.J., 1988, The formation of areally-averaged roughness lengths. *Quart. J. Roy. Meteorol. Soc.*, **114**, 399–420.

McNaughton, K.G., 1994. Effective stomatal and boundary layer resistances of heterogeneous surfaces. *Plant Cell Environ.*, **17**, 1061–1068.

Monteith, J.L., 1965. Evaporation and the environment. Symposium of Society of Experimental Biology, **19**, 205–234.

Noilhan, J. and Lacarrere, P., 1995, GCM grid scale evaporation from mesoscale modelling. *J. Climate*, **8**, 206–223.

Pinker, R.T. and Ewing, J.A., 1985. Modelling surface radiation: model formulation and validation. *J. Climate Appl. Meteorol.*, **24**, 389–401.

Pinker, R.T. and Laszlo, I., 1990. Improved prospects for estimating insolation for calculating regional evaporation from remotely sensed data. *Agric. For. Meteorol.*, **52**, 227–251.

Pinker, R.T. and Laszlo, I., 1992. Modelling surface solar irradiance for satellite applications at global scale. *J. Appl. Meteorol.*, **31**, 194–211.

Pinker, R.T. Kustas, W.P. Laszlo, I. Moran, M.S. and Huete, A.R., 1994. Basin-scale solar irradiance estimates in semi-arid regions. *Wat. Resour. Res.*, **30**, 1375–1386.

Raupach, M.R., 1995. Vegetation-atmosphere interaction and surface conductance at leaf, canopy and regional scales. *Agric. For. Meteorol.*, **73**, 151–179.

Raupach, M.R. and Finnigan, J.J., 1995. Scale issues in boundary-layer meteorology: surface energy balances in heterogeneous terrain. *Hydrol. Processes*, **9**, 589–612.

Raupach, M.R. and Finnigan, J.J., 1997. The influence of topography on meteorological variables and surface-atmosphere interactions. *J. Hydrol.*, **190**: 182–213.

Reed, B.C., Brown, J.F. VanderZee, D. Loveland, T.R. Merchant, J.W. and Ohlen, D.O., 1994. Measuring phenological variability from satellite imagery. *J. Veg. Sci.*, **5**, 703–714.

Running, S.W., Justice, C.O. Salomonson, V. Hall, D. Barker, A.J. Kaufmann, Y.J. Strahler, A.H. Huete,A.R. Muller, J-P. Vanderbilt, V. Wan, Z.M. Teillet, P. and Carneggie, A.D., 1994. Terrestrial remote sensing science and algorithms planned for EOS/MODIS. *Int. J. Remote Sens.*, **15**, 3587–3620.

Sellers P.J., Mintz, Y. Sud, Y.C. and Dalcher, A., 1986. A Simple Biosphere Model (SiB2) for use with General Circulation Models. *J. Atmos. Sci.*, **43**, 6505–531.

Sellers P.J., Randall, D. Collatz, J. Berry, J. Field, C. Dazlich, C. Zhang, C. Collelo, G. and Bounous, A., 1996a. A revised land surface parameterization (SiB2) for atmospheric GCMs: model formulation: part I. *J. Climate*, **9**, 676–705.

Sellers P.J., Los, S.O. Tucker, C.J. Justice, C.O. Dazlich, D.A. Collatz, G.J. and Randall, D.A., 1996b. A revised land surface parameterization (SiB2) for atmospheric GCMS. part II: the generation of global fields of terrestrial biophysical parameters from satellite data. *J. Climate*, **9**, 706–737.

Shuttleworth, W.J., 1991. The Modellion Concept. *Reviews of Geophysics*, **29**, 585–606.

Shuttleworth, W.J., Yang, Z.-L. and Arain, M.A., 1997. Aggregation rules for surface parameters in global models, *Hydrol. Earth System Sci.*, **2**, 217–226.

Stauffer, D.R., and Seaman, N.L., 1990. Use of four-dimensional data assimilation in a limited area model. Part I: experiments with synoptic-scale data. *Monthly Weather Rev.*, **118**, 1250–1277.

Toth, J.J., Moran, M.S. Goodrich, D. and Avissar, R., 1998. Coupling Landsat data with a mesoscale model to estimate evapotranspiration, submitted to *J. App. Meteorol.*

Wieringa, J., 1986. Roughness dependent geographical interpolation of surface wind speed averages, *Quart. J. Roy. Meteorol. Soc.*, **112**, 867–889.

# Appendix: List of Symbols

$A$ available energy for the whole model grid
$A_i$ available energy for pixel $i$
$A_m$ available energy for the whole model grid in the 4DDA model
$A'_m$ available energy for cloud-free pixels in the 4DDA model
$c_p$ isobaric specific heat of air
$d$ zero plane displacement for the whole model grid
$d'$ effective zero plane displacement for the cloud-free portion of the grid
$D$ [$= q_{sat}(\theta) - q$] potential saturation deficit of ambient air at blending height
$E$ average latent heat flux for the whole model grid
$E_i$ latent heat flux for pixel $i$
$E_m$ average model-calculated latent heat flux for the cloud-free portion of the grid
$F$ generic function relating aerodynamic resistance for energy transfer to that for momentum transfer
$H$ sensible heat flux for the whole model grid
$H'$ sensible heat flux for the clear-sky pixels in the grid square
$H_i$ sensible heat flux for pixel $i$
$H'_m$ sensible heat flux for the clear-sky pixels in the 4DDA model
$i$ pixel number in grid square
$l$ generic function describing relationship between surface resistance and leaf area index
$L_n$ net longwave radiation for the whole model grid
$L_{n,m}$ net longwave radiation for the whole model grid calculated by the 4DDA model
$L_i$ leaf area index of the pixel $i$
$M'_s$ improved soil-moisture estimate for successive iterations
$Ms$ available soil moisture in the 4DDA model
N number of pixels in the grid square
q specific humidity at blending height
$q_{sat}(T)$ saturation specific humidity as a function of temperature T
$r_{a,i}$ aerodynamic resistance for energy transfer for pixel $i$
$r_{a,M,i}$ aerodynamic resistance for momentum transfer for pixel $i$
$r_{s,i}$ surface resistance for pixel $i$
$R_a$ aerodynamic resistance for energy transfer for the whole model grid
$R'_a$ effective aerodynamic resistance for energy transfer for the cloud-free pixels
$R_{a,M}$ aerodynamic resistance for momentum transfer for the whole model grid
$R'_{a,M}$ effective average aerodynamic resistance for momentum transfer for the cloud-free pixels
$R'_s$ effective surface resistance for the cloud-free pixels
$R_s$ surface resistance for the whole model grid
$S$ average downwelling solar radiation for the whole model grid
$S'$ downwelling surface solar radiation within radiation algorithm in cloud-free conditions
$S_{n,m}$ average net solar radiation for the whole model grid calculated by the 4DDA model
$t$ generic function relating aerodynamic surface temperature to remotely sensed surface temperature for pixel $i$
$T_{s,a,i}$ 'aerodynamic' surface temperature for pixel $i$
$T_{s,R,i}$ remotely sensed surface temperature for pixel $i$
$U_b$ average wind speed predicted at the blending height in the 4DDA model
$w_i$ fractional area of pixel $i$
$z_b$ blending height (often taken as the lowest model level)
$z_0$ aerodynamic roughness length for the whole model grid
$z'_0$ effective aerodynamic roughness length for the cloud-free portion of the grid
$\alpha$ albedo for pixel $i$
$\delta_i$ [= 1] for cloud-free pixels, [ = 0] for pixels partially or wholly covered by cloud
$\Delta$ [$= (\lambda/c_p)\, dq_{sat}/dT$] dimensionless slope of the saturation specific humidity
$\kappa$ von Karman constant
$\lambda$ latent heat of vaporisation of water
$\theta$ potential temperature at blending height
$\rho$ air density