Environmental Modeling of Physical, Biophysical and Chemical Processes in the Atmosphere Plant- Soil- Interaction: How Nonlinearity Affects the Solutions?

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Abstract: An experience with numerical modeling of biophysical and chemical processes at the land-atmosphere interface has progressed over the decades. The environmental modeling community has come to recognize that various aspects of atmosphere-ecosystem-ocean system that once were thought to play a relatively minor role are actually very important in the biophysical and chemical dynamics and circulations of the lower part atmosphere environment. Ecosystem and soil-plant-atmosphere processes and their effect on the atmosphere are certainly in this category. In providing a reliable sophisticated information, either for scientific or operational purposes, the environmental models dealing with the foregoing processes still meet with methodological, mathematical as well as software problems. The objective of this paper is to give the overview some of problems in environmental modeling of physical, biophysical and chemical processes in the soil-plant-atmosphere interactions related to chaotic behavior and problem of realisability.

Keywords: Environmental modeling; Modeling of biophysical and chemical processes in land surface-atmosphere interaction; Parameters aggregation; Flux aggregation; Nonlinear processes; Deterministic chaos; Realisability conditions.

1. INTRODUCTION

Many complex environmental problems of small, medium or large scales involve processes that occur both within and between environmental media (e.g., air, surface water, groundwater, soil, and biota). For example, when styling the origin, transport, and fate of photochemical oxidants in the atmosphere, the interaction of atmospheric constituents and land cover is important. Similarly, water quality in a river is affected by meteorology, air quality, soil composition, vegetation type, land use, vehicles, and contiguous water bodies. Recently, there has been an increasing demand for providing a high level of production of wholesome plant food but without losing its quality from the customer's point of view. In this regard, it is required to provide reliable information about occurrence of plant diseases so as to ensure their efficient control using properly balanced meteorological and biometeorological information. Also, increasing number of studies of the rate of spread of fires have revealed a definite need for better understanding of the behavior of wind, especially inside and above the forest. Therefore, the processes occurring both within and between environmental media must be investigated, understood, and modeled [Brandmeyer and Karimi, 2001]. There is considerable recent research work that demonstrates the different aspects of modeling of processes within and between environmental media using new approaches, numerical and software techniques [Mihailovic and Kallos, 1997; Janjic, 1998; Mihailovic, et.

al, 2001a; Mihailovic et al., 2001b; Lalic and Mihailovic, 2002; Mihailovic et al., 2002a].

There are several groups of short (biophysical), medium (biogeochemical), and long-term (biogeographic) effects of landscape processes on weather and climate that play the vital role. Thus, biophysical effects include, for example, the influence of transpiration on the ratio of sensible and latent turbulent fluxes in the surface heat budget. Biogeochemical effects include the growth of plants, which alter the amount of transpitrating leaf surface, and surface albedo, as well as the storage of carbon. Biogeographic influences involve the alternation of vegetation species composition over time [Rodhe, 2000; Pielke, 2002]

In providing a reliable sophisticated information, either for scientific or operational purposes, the environmental models dealing with the foregoing processes presently still meet with methodological, mathematical as well as software problems. The landscape directly and indirectly determines the ground's energy budget through biophysical, biogeochemical, biogeographic effects. Since landscape (and other atmosphere - surface interactions) involve complex nonlinear feedbacks, accurate prediction of environmental variables, such as temperature, precipitation, soil moisture, and vegetation growth beyond, etc. cannot be achieved because of the occurrence of some uncertainties. They occur through the non-linearity of the relationship between turbulent fluxes and vertical mean profiles as well as the chaotic time fluctuations of ground surface temperature resulting from the energy balance equation applied for the ground surface - atmosphere system [Mihailovic et al., 2001]. In this paper we will briefly discuss these problems. Firstly, we will consider an example of energy balance leading to chaotic behavior of ground surface temperature under some conditions. Secondly, we will suggest a combined method for calculation of key variables for determining the energy and momentum exchanges between the grid cell of underlying surface and atmosphere.

2. THE CHAOTIC TIME FLUCTUATIONS OF GROUND SURFACE TEMPERATURE

Current numerical modelers in environmental studies still base their calculations on the traditional mathematical models of dynamical systems, whose time evolution is described by the Newtonian continuum dynamics leading to nonlinear partial differential equations for relevant environmental quantities. These differential equations generally do not have analytical solutions, so one has to use numerical methods, which can be sensitive to initial conditions. However, small "tuning" of initial conditions can conduct the numerical model to instability if the system is a chaotic one. In this paper we present an illustrative example of such behavior in an important environmental system where an interface occurs.

The system considered is the atmosphere interacting with soil surface and the quantity exhibiting the chaotic behavior is the ground temperature. To demonstrate that let us consider the energy balance equation over a bare soil containing a large amount of water, i.e., when it is in the potential evaporation regime and when the sky is completely covered by clouds. In that case the sensible heat flux as well as the soil heat flux can be both safely neglected while the net radiation is treated in the linear approximation. Under these conditions the energy balance equation can be written in the form:

$$C_g \frac{\partial T_g}{\partial t} = a\left(T_g - T_a\right) - \frac{c_p \rho}{\gamma} \frac{E(T_g) - e_a}{r_* + r_a} \qquad (1)$$

where C_g is the ground heat capacity, t is time, T_g is the ground surface temperature, a is a constant, T_a the air temperature at reference level, c_p is the specific heat of air at constant temperature, ρ is the air density, γ is the psychrometric constant, $E(T_g)$ is the saturated vapor pressure at ground surface temperature, e_a is the vapor pressure at reference level, r_* is the surface resistance and r_a is the aerodynamic resistance. For the foregoing ambient conditions, it can be assumed that: (a) there is no large variation in the diurnal course of air temperature ($T_a \approx$const.), the air is nearly saturated, i.e. e_a is quite close to $E(T_a)$ and (c) there is no large difference between ground surface and air temperature, i.e. $T_a \approx T_g$. Under the last condition the relationship between the saturated vapor pressures $E(T_g)$ and $E(T_a)$ can be written as $E(T_g) \approx E(T_a) exp(b(T_g - T_a))$ where b=0.0670 °C^{-1} for temperatures around 20 °C. After expanding expression for $E(T_g)$ in Taylor's series and its substitution in Eq. (1) we get

$$\frac{\partial \tau}{\partial t}=\frac{a-AbE(T_a)}{C_g}\tau-\frac{Ab^2E(T_a)}{2C_g}\tau^2 \qquad (2)$$

where $A = c_p\,\rho/(\gamma(r_* + r_a))$ and $\tau = T_g - T_a$. If we write Eq. (2) in the finite difference form and introducing a time step Δt and number of step n we reach the so called "logistic" equation having the form

$$\Gamma_{n+1} = B\Gamma_n(1-\Gamma_n) \qquad (3)$$

where the quantity Γ_n is defined as $C\tau_n/B$ while the symbols introduced have the following meaning:

$$B=\frac{a-AbE(T_a)}{C_g}\Delta t+1$$

and

$$C=\frac{Ab^2E(T_a)}{2C_g}\Delta t\,.$$

Eq. (3) leads to chaotic behavior [Feigenbaum, 1984]. Figure 1 depicts irregular behavior of Γ including difference between ground surface and air temperature for initial condition $\Gamma = 0.001$ and $B = 3.3$. It seems that the foregoing relatively simple realistic assumptions introduce the chaotic behavior resulting in ground surface temperature fluctuations, which create problems in running the environmental models.

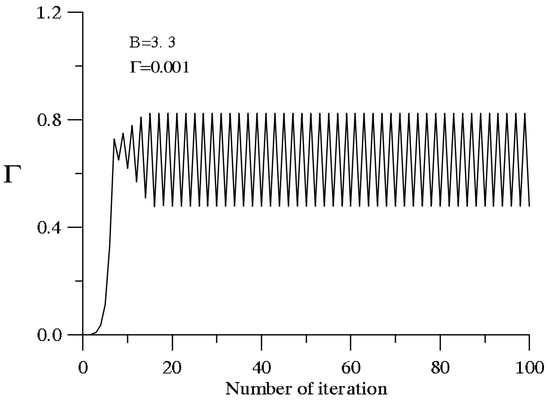

Figure 1. Irregular behavior of dimensionless quantity Γ expressing difference between ground surface and air temperature.

3. AGGREGATION OF FLUXES AND PARAMETERS OVER GRID CELL: REALISABILITY CONDITIONS

It is well known that turbulent transfer models can sometimes produce results that cannot be realized in nature. This situation is particularly important in the case of parameterization of land-surface turbulent transfer over heterogeneous surfaces. An improper parameterization of land-surface processes leads to uncertainties in calculating the boundary layer variables and further in predicting the temperature and other meteorological quantities in environmental models. For example, a detailed overview of the literature related to the problems faced when determining momentum and energy fluxes over heterogeneous surfaces is comprehensively given in Burke et al. [2000]. In the numerical modeling of surface layer processes, three approaches are commonly taken for calculating the transfer of momentum, heat and moisture from a grid cell comprised of heterogeneous surfaces. According to Hess and McAvaney [1997, 1998] they are: (a) "parameter aggregation", where grid cell mean parameters such as roughness length, albedo, leaf area index, stomatal resistance, soil conductivity, etc., are derived in a manner which attempts to best incorporate the combined nonlinear effects of each of different relatively homogeneous subregions ("tiles") over grid cell; (b) "flux aggregation", where the fluxes are averaged over the grid cell, using a weighted average with the weights determined by the area covered by each tile; and (c) a combination of the flux aggregation and parameter aggregation methods [Claussen, 1991; Claussen, 1995].

When the parameter aggregation method is applied (which creates an "effective" homogeneous surface) then we meet with the question of its physical realisability. It will be realisable as long as the surface layer temperature and specific humidity gradients that result from the aggregation have the same sign as the fluxes of latent and sensible heat fluxes, respectively. However, when either the flux aggregation method or its combination with the parameter aggregation is used then certain anomalies can arise through the occurrence of the "Schmidt paradox" (see the discussion by Claussen [1991]). Shortly, it can be described in the following manner. Small regions of strong turbulence in unstable conditions can dominate the grid-area averaged fluxes, but have less effect on the vertical mean value of the gradient between the surface and the lowest level model, leading to a situation of counter-gradient transport.

Following the foregoing context about the physical realisability when the aggregation parameter method is applied it is clearly seen that it is strongly influenced by the reliability of method for calculating the “effective“ temperature of homogeneous surface. Consequently, it is useful to examine the difference of two methods commonly used in calculating the “effective“ temperature over the grid-cell consisting of different fraction of underlying surface. Since more uncertainties in the turbulent fluxes exchanges between such designed grid cell and above air layer are expected, we have performed a numerical experiment with the forcing atmospheric data at 10 m level.

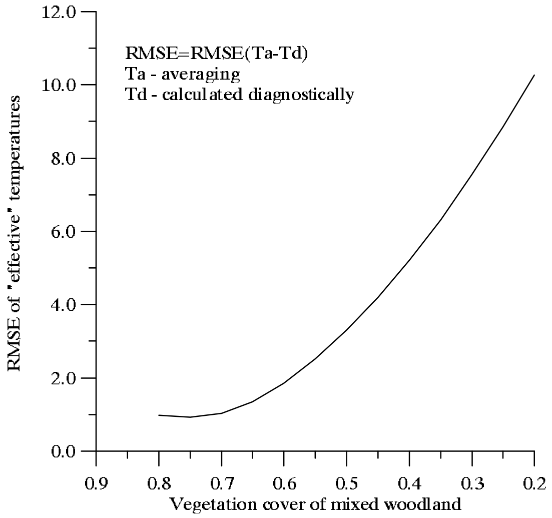

Figure 2. The RMSE between the values of "effective" surface temperature obtained by two methods for different fraction of forest canopy in the grid cell.

We assume that single grid cell consists of two different covers commonly appearing as land-use categories in grid cells in environmental models, i.e. bare soil and mixed woodland. Calculations have been performed by the LAPS scheme [Mihailovic et al., 2002a], using two methods for calculating the “effective“ temperature as a function of fractional covers of two different patches, whose impact as a whole is considered in the following manner. When a fractional cover σ of the first patch of a grid cell is chosen to be independent variable (bare soil), increasing in the range from 0 to 1, the fractional cover of the second patch (mixed woodland) automatically has taken, value set to be ($1-\sigma$). In the first method the “effective“ temperature of the grid cell is calculated as a simple average of bare soil and mixed woodland surface temperatures, while in the second method it is determined diagnostically from the energy balance equation. This equation represented the equality of the sensible heat flux from the canopy to some reference level in the atmosphere and the sum of sensible heat flux from the ground and sensible heat flux from the leaves to the canopy air volume (Mihailovic et al., 2002a). In experiments, we used the mixed woodland, (fractional cover σ = 0.87 and an average height of 13 m) growing over the loamy sand soil. The other morphological, physiological and soil parameters are taken from Mihailovic and Kallos [1997]. The volumetric soil water content in soil layers: 0.1 m, 0.4 m and 1.0 m initially had the values of 0.18 m^3m^{-3}, 0.19 m^3m^{-3} and 0.20 m^3m^{-3}. Differences in the numerically simulated values of “effective“ temperature produced by changes in fraction of the vegetation in the grid cell were quantified by the root-mean-square-error (RMSE) between them (Figure 2). Looking at this figure it is seen that for higher fraction values of vegetation, the RMSE is lower for both the vegetative covers crop and mixed woodland. Expectantly, the lower fraction of bare soil does not significantly contribute to the sensible heat fluxes directed from the grid cell into atmosphere. It means that small changes in fractional cover of vegetation do not produce significant changes in “effective“ temperature regardless of the method applied. However, the increasing of the bare soil fraction leads to fast growth temperatures reaching the value of 10 ^{0}C when fractional cover is around. This is due to the fact that evapotranspirational cooling of the grid cell becomes smaller while the sensible heat flux from the bare soil takes the main role in the land atmosphere energy exchange resulting in a higher error in calculating the “effective“ temperature. However, according to Hess and McAvaney [1998], it seems that averaging temperatures over different patches, rather than the sensible heat flux, can be the source of problems.

Mihailovic et al. [2002c] recommended an alternative method for calculating the quantities including the momentum, heat and water exchange expressions, i.e. friction velocity u_*, surface temperature T_0 and water vapor pressure e_0, when the averaged flux over the grid cell consisting of different patches is known. They found the following expressions:

$$\left\langle u_*^2 \right\rangle = \sum_i \sigma_i \left[\frac{k\Lambda_i}{\ln \frac{z_a - D_i}{Z_{0,i}}} \right]^2 u_a^2 , \qquad (4)$$

$$\left\langle T_0 \right\rangle = \frac{\ln \frac{z_r - \langle D \rangle}{\langle H \rangle - \langle D \rangle} \left\langle H_0 \right\rangle}{\rho c_p k\Lambda \left\{ \sum_i \sigma_i \left[\frac{k\Lambda_i}{\ln \frac{z_a - D_i}{Z_{0,i}}} \right] \right\}^{1/2} u_a} + T_a \qquad (5)$$

and

$$\left\langle e_0 \right\rangle = \frac{\gamma \ln \frac{z_a - \langle D \rangle}{\langle H \rangle - \langle D \rangle} \left\langle \lambda E_0 \right\rangle}{\rho c_p k\Lambda \left\{ \sum_i \sigma_i \left[\frac{k\Lambda_i}{\ln \frac{z_a - D_i}{Z_{0,i}}} \right] \right\}^{1/2} u_a} + e_a . \qquad (6)$$

In the last three equations we used angular brackets to indicate an average over the grid cell for canopy height (H), latent heat flux (λE_0) and sensible heat flux (H_0) and displacement height (D) while Λ is a dimensionless aerodynamic parameter in the wind profile expression introduced by Mihailovic et al [2002b]; λ is the latent heat of vaporization, while subscript a indicates the values of air temperature (T), water vapor pressure (e) and wind speed (u) at reference level (z_a). $Z_{0,i}$ and D_i are generalized values of roughness lengths and displacement height of the ith grid cell patch having fractional cover σ_i [Mihailovic et al., 1999]. If the momentum flux is determined by the flux-aggregation and the sensible and latent heat fluxes are found combining the flux and parameter aggregation, then the sign of the sensible heat flux and the "surface" temperature gradient should agree and the "surface" temperature is found from Eq. (5). Similarly, the grid-averaged vapor pressure is determined by Eq. (6) providing the realisability.

4. CONCLUDING REMARKS

Current numerical modelers in environmental studies still base their calculations on the traditional mathematical models of dynamical systems, whose time evolution is described by the Newtonian continuum dynamics leading to nonlinear partial differential equations for relevant environmental quantities whose solutions can result in a chaotic behavior under some conditions. Also, environmental models can sometimes produce results that cannot be realized in nature. This situation is typically met in modeling of surface layer processes as well as in calculating the transfer of momentum, heat and moisture over the grid cell consisting of heterogeneous surfaces. Depending on the method applied, the problem of realisability conditions will occur. We considered the application of energy balance equation over the bare soil largely supplied by the water and with the high

Amount of cloudiness in meteorological conditions. Under these conditions this equation can turn into the "logistic" equation leading to chaotic behavior of difference between the surface ground and air temperature. Also, we suggested an alternative method for determining the surface temperature and water vapor pressure and friction velocity over the heterogeneous grid cell combining the flux and parameter aggregation. This method is physically realisable since the sign of the surface flux agrees with the surface gradient.

5. ACKNOWLEDGEMENTS

This research was supported by the New York State Energy Research and Development Authority contract No. 4914-ERTER-S99 awarded to Dr. S.T. Rao of the University at Albany.

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