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MATHEMATICAL MODELS AND SOLUTION TYPES IN THE ATMOSPHERIC BOUNDARY LAYER PHENOMENA

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Abstract. Recently it is recognized the crucial importance of rigorous mathematical investigation in meteorology. In this context the atmospheric boundary layer models give a special type approximation related to the order of the functions implied in these problems. The present paper points out on some directions of approximate investigations of these types of models, and aims to approach the optimum between some numerical software appliances.

1. Introduction: Phenomenology of the atmospheric planetary boundary layer

The state of the atmosphere has affected human activities since time immemorial. Since the 1950s, when the first successful attempt to foresee future development of weather using the solution to the equations describing the atmosphere behavior, the numerical weather prediction has become broadly used almost in all weather services around the world. Our knowledge about the atmosphere is ever evolving process and possible way that helps to maintain to keep this active is the mathematical modeling of the atmospheric processes. A lot of processes are implied, from classical hydrodynamics to quantum physics, numerical mathematics, chemistry (especially related to air pollution). It is necessary to emphasize that many processes in the atmosphere are of a nonlinear nature and they show, in many cases, a chaotic behavior (for example turbulence) that makes their description and modeling quite complicated. In classical fluid dynamics, a boundary layer is the layer in a nearly inviscid fluid next to a surface in which frictional drag associated with that surface is significant (term introduced by Prandtl in 1905). Such boundary layers can be *laminar* or *turbulent*, and are often only mm thick. In the atmospheric science there is a similar definition: the Atmospheric Boundary Layer (ABL), sometimes called Planetary (PBL) is the layer of fluid directly above the Earth's surface in which significant fluxes of *momentum, heat* and/or *moisture* are carried by turbulent motions whose horizontal and vertical scales are on the order of the boundary layer depth, and whose circulation timescale is a few hours or less (Garratt 1994a,b).

The complexity of this definition is due to the complicated processes of aerodynamics:

1. *Surface heat exchange can lead to thermal convection*
2. *Moisture and effects on convection*
3. *Earth's rotation*
4. *Complex surface characteristics and topography.*

Generally the BL models include the study of fluxes of heat, moisture and momentum between the atmosphere and the underlying surface, and how to characterize surfaces so as to predict these fluxes (roughness, thermal and moisture fluxes, radiative characteristics). The PBL characteristics can be synthesized in the following figure:

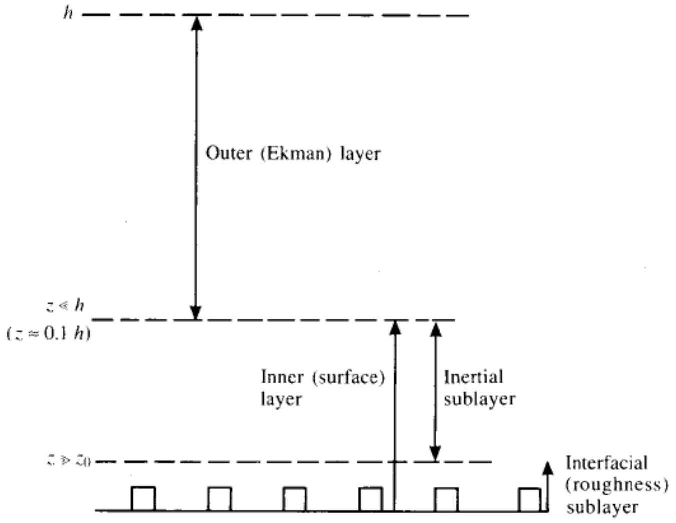

FIGURE 1. The component layers of the PBL.

1. Interfacial sublayer - in which molecular viscosity/diffusivity dominate vertical fluxes
2. Inertial layer - in which turbulent fluid motions dominate the vertical fluxes, but the dominant scales of motion are still much less than the boundary layer depth. This is the layer were most of surface wind measurements are made. The above two layers comprise the surface layer. Coriolis phenomenon turning of the wind with height is not evident within the surface layer.
3. Outer layer - the layer of turbulent fluid motions with scales of motion comparable to the boundary layer depth (where the so-called *large eddies* appear).

The figures 2 and 3 below give a intuitive presentation for the symbolic structure of the atmosphere. The troposphere can be divided into two parts: a boundary layer (blue) near the surface and the free atmosphere above. The PBL can be subdivided into four separate component layers: the surface layer, the mixed layer, the stable layer, and the residual layer. All these can be easily observed in the figures below.

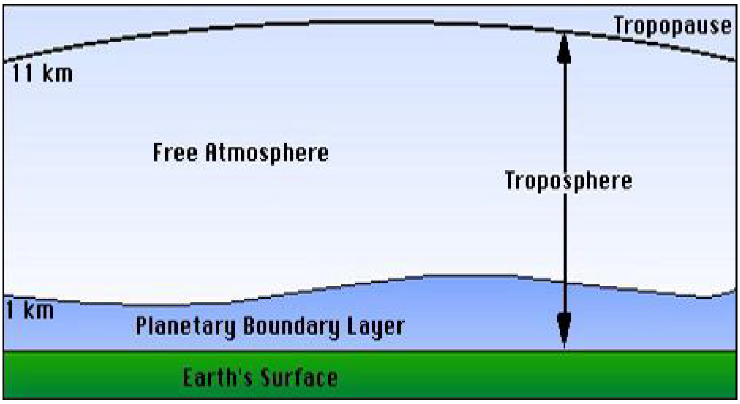

FIGURE 2. The troposphere structure.

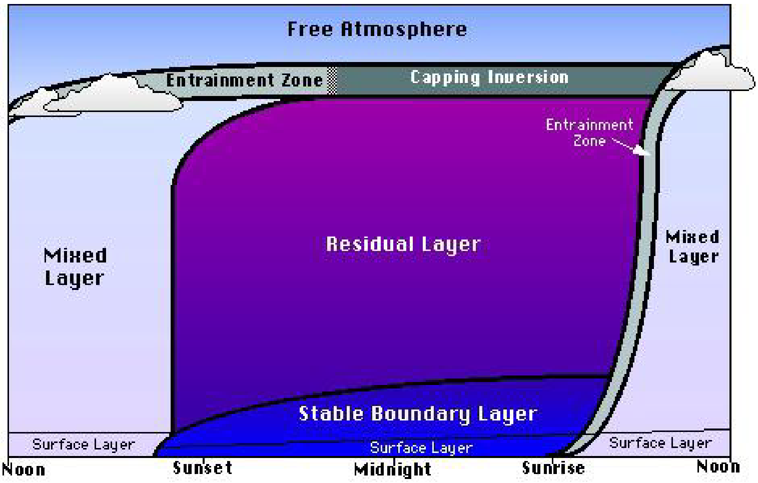

FIGURE 3. The four component layers.

2. Averaging in PBL mathematical framework

The boundary layer is the part of the atmosphere in which we live and carry out most human activities. Moreover, almost all exchange of heat, moisture, momentum, naturally occurring particles, aerosols, and gasses, and pollutants occurs through the BL. Five basic applications of the PBL features are as follows.

i Climate simulation - parametrization of surface characteristics, air-surface exchange, BL thermodynamics fluxes and friction, and cloud. No climate model can succeed without some consideration of the boundary layer
ii Air Pollution and Urban Meteorology - Pollutant dispersal, interaction of BL with meso-scale circulations. Urban heat island effects
iii Agricultural meteorology - Prediction of frost, dew, evapo-transpiration
iv Aviation - Prediction of fog formation and dissipation, dangerous wind-shear conditions
v Remote Sensing - Satellite-based measurements of surface winds, skin temperature, etc. Involve the interaction of BL and surface, and must often be interpreted in light of a BL model

2.1. Turbulence. Spectral gap. We generally associate the slowly-varying quantities as corresponding to the synoptic-scale, whereas the turbulent fluctuations are due to small-scale processes. This distinction between mean flow and turbulence is justified by the existence of a spectral gap, a region in frequency space in which there is relatively little variability on time scales between about 10 minutes (turbulence scales) and 10 hours (synoptic scales). The figure 4 below shows a classical spectral gap (Holton 2004).

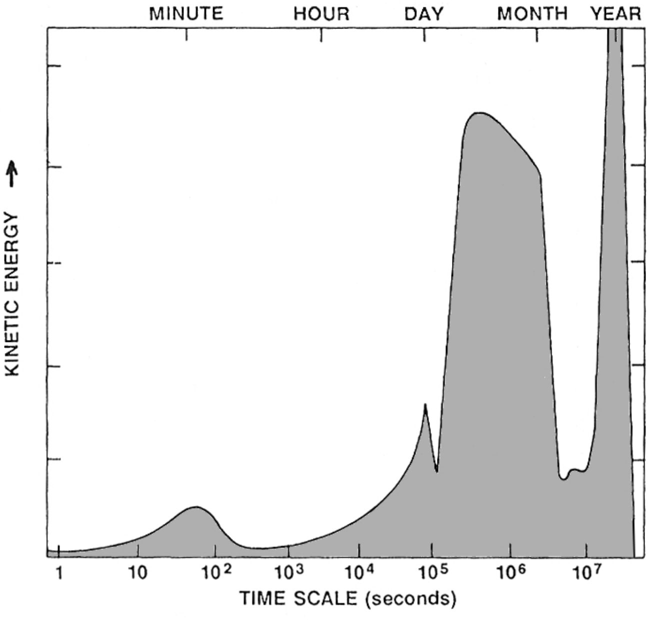

FIGURE 4. Spectral gap.

The spectrum shows four obvious energy peaks. The peaks at one day and one year are the diurnal and annual cycles. The peak that occurs between one day and one month is associated with *baroclinic instability* in the mid-latitude westerlies. The peak at about one minute is associated with *atmospheric turbulence* and *convection*. It is important to notice that there appears to be a lack of energy having time periods of about 30 min to 1 h. This is the so-called *spectral gap* which is very important for the derivation of turbulent kinetic energy (TKE) equation.

2.2. Mean part. Turbulent part. Modeling the turbulent flows is an important part of applied mathematics and in the meantime of fluid dynamics (Henson and Seborg 2005; Wilcox 2006). The method of separation the turbulent from non-turbulent flow is signal averaging over a period of 30 min to 1 h. That's how we can separate turbulent scale motions from non-turbulent scale motions. The non-turbulent part of the flow is represented by the equation

$$\bar{A}(s) = \frac{1}{T}\int_0^T A(t,s)dt \tag{1}$$

where T is some value in the time interval of spectral gap, so 30 min to 1 h. Here s is some other spatial variable and A is variable like temperature or velocity field. Once we have the mean (non-turbulent) part of the signal $\bar{A}$, we can substract it from the actual signal (A) to get the turbulent part of the signal (a'):

$$a' = A - \bar{A} \tag{2}$$

and thus we can separate the turbulent and non-turbulent part. From the equations (1), (2) it's obvious that this kind of averaging is not so good for motions of scales of about 1 h, but for larger scales of turbulence. Still, because of existence of spectral gap this is not a problem, since there is no motions at those scales, therefore this method of separation works.

If A and B are two variables dependent on time, and c is a constant, some basic rules of averaging are as follows:

$$\overline{c} = c, \quad c\overline{A} = \overline{cA}, \quad \overline{\overline{A}} = \overline{A}, \quad \overline{A+B} = \overline{A} + \overline{B}, \quad \overline{\overline{A}B} = \overline{A}\,\overline{B} \tag{3}$$

.

2.3. Reynolds averaging. The above averaging rules can now be applied to variables that are split into mean and turbulent parts. Let two quantities A and B be like in the equation (2) above:

$$A = \overline{A} + a', \quad B = \overline{B} + b' \tag{4}$$

.

We have the following relation:

$$\overline{A} = (\overline{\overline{A} + a'}) = \overline{\overline{A}} + \overline{a'} = \overline{A} + \overline{a'} \tag{5}$$

So, the right and left sides are equal only if the turbulent part equals zero, $a' = 0$, which is not surprising because of the meaning of the equation (1). The similar works for the terms $\overline{\overline{A}b'} = \overline{\overline{B}a'} = 0$.

The importance of Reynolds averaging consists in few formula which will lead us to the concept of eddy or turbulent flow, as follows. The basic formula is given by:

$$\overline{AB} = (\overline{\overline{A}+a') + (\overline{B}+b'}) = (\overline{A})(\overline{B}) + \overline{a'b'} \tag{6}$$

.

The non-linear product $\overline{(a'b')}$ is not necessary equal to zero - and similar $\overline{a'^2}$ $\overline{b'^2}$. This is because they have similar meaning with the important statistical measures:

(1) the dispersion: $\sigma_A^2 = \frac{1}{n}\sum_{i=0}^{n-1}(A_i - \bar{A})^2 = \overline{a'^2}$

(2) the covariance: $covar(A,B) = \frac{1}{n}\sum_{i=0}^{n-1}(A_i - \overline{A}(B_i - \overline{B}) = \overline{a'b'}$

Therefore they could be zero in some selected cases. Such variable $\overline{a'b'}$ is named or turbulent flux and is of primary importance for understanding turbulence. Let us consider the velocity field U_i, $i = 1,2,3$, $U_i = \overline{U_i} + U_i'$ and A some variable, $A = \overline{A} + a'$. We have the following relations:

$$\begin{aligned} \frac{dA}{dt} &= \frac{\partial A}{\partial t} + U_i \frac{\partial A}{\partial x_i} \\ &= \frac{\partial(\overline{A}+a')}{\partial t} + (\overline{U_i} + U'_i)\frac{\partial(\overline{A}+a')}{\partial x_i}\frac{(d\overline{A})}{dt} \\ &= \frac{\partial \overline{A}}{\partial t} + \overline{U_i}\frac{\partial \bar{A}}{\partial x_i} + \left(\overline{U_i}\frac{\partial a'}{\partial x_i}\right) \end{aligned} \tag{7}$$

where the Einstein summation convention is used. In the last equation in (7) the additional term represents the advection of a' with u'. Using the continuity equation where we assume incompressibility we get the following implications:

$$\frac{\partial U_i}{\partial x_i} = 0 \Rightarrow \frac{\partial \bar{U}_i}{\partial x_i} = 0 \Rightarrow \frac{\partial U_i'}{\partial x_i} = 0 \tag{8}$$

If we multiply the last equation from system (8) with a' and add to $\frac{d\bar{A}}{dt}$ we get

$$\frac{d\bar{A}}{dt} = \frac{\partial \bar{A}}{\partial t} + \overline{U_i}\frac{\partial \bar{A}}{\partial x_i} + \frac{\partial \overline{(a'u_i')}}{\partial x_i} \tag{9}$$

So, the total derivative consists of two parts. The first one is just the total derivative of $\bar{A}$, where the advection is driven by $\bar{U}_i$. The second part is the advection of a' driven by U_i' and it can be described as the divergence of turbulent momentum flux. Thus, when we want to calculate the average part of total derivative of A we also need to know something about turbulence. That means, *the mean flow is directly influenced by turbulence*.

It is known that fluid motion can transport quantities, therefore turbulence (turbulent flux) can transport quantities, too. This mechanism is presented by terms which are similar with $\overline{(a'b')}$. When the eddy flux (turbulent flux) is defined by $\overline{(w'\Theta')}$, we get the so-called heat turbulent flux. Here w' is the turbulent part of the velocity and Θ' is the turbulent part of potential temperature, given by

$$\theta = T(\frac{p_0}{p})^{\frac{R}{c_p}} \tag{10}$$

where T is the current absolute temperature in the parcel (measured in Kelvin deg), R is the gas constant of air, and c_{rho} is the specific heat capacity at a constant pressure. A line of constant Θ presents where dry air particle can move. If turbulence is completely random, then a positive $\overline{(w'\Theta')}$ at one instant might cancel a negative $\overline{(w'\Theta')}$ at some later instant, resulting in a near zero value for average turbulent heat flux. But there are situations where the average turbulent heat flux might be significantly different from zero.

2.4. The conservation of momentum. With the above framework related to Reynold averaging and eddy flux, we can step next to the turbulent kinetic energy (Zdunkowski and Bott 2012). In order to derive turbulent kinetic energy equation, it is necessary to start with Newton's second law. The basic form is:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\delta_{i3} g - 2\varepsilon_{ijk}\Omega_j U_k - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} \tag{11}$$

where: $U_i = \bar{U}_i + U_i'$ is the velocity field, denoted in three dimensional space, as usual: $U_1 = U_x = u U_2 = U_y = v U_3 = U_z = w$; δ_{ij} is the Kronecker delta; ε_{ijk} is the alternating unit tensor; p is the pressure, ρ is the density and τ_{ij} is the stress. In the very basic form of the (11) we have the following representations for the equation' s components:

(1) The first term represents the *storage* of momentum
(2) The second term represents the *advection* of momentum
(3) The third term – the *pseudo-gradient* forces
(4) The fourth – the influence of *viscous stress*

It is important to notice that the first and fourth terms can be simplified. The first one is often written as $f\varepsilon_{ij3}U_j$ with $f = 2\omega sin\varphi$ the Coriolis parameter, and $\omega = \frac{2\pi}{24}\frac{1}{h}$. The fourth term (which is more complicated) can reduce to $\frac{\mu}{\rho}\frac{\partial\partial U_i}{\partial x_j^2}$.

2.5. The turbulent kinetic energy (TKE). The idea for the definition of the turbulent kinetic energy (TKE) is very similar to the idea of kinetic energy. Let $\vec{U}$ be the velocity field. Then we can define $\vec{U} = \vec{\overline{U}} + \vec{U}'$ like in equation (2). We can define two kinds of kinetic energy:

$$\frac{MKE}{m} = \frac{1}{2}((\overline{u})^2 + (\overline{v})^2 + (\overline{w})^2) \tag{12}$$

which is the kinetic energy of the mean flow;

$$\frac{TKE}{m} = \bar{e} = \frac{1}{2}((\overline{u}')^2 + (\overline{v}')^2 + (\overline{w}')^2) \tag{13}$$

which is the kinetic energy of turbulent part of the flow. Turbulent kinetic energy is one of the most important variables in micro-meteorology. It's a measure of the intensity of turbulence. The turbulence may change in time, therefore an interes is given in TKE to the budget equation $\frac{\partial\bar{e}}{\partial t}$ (as presented in Holton (2004)). The total changes in TKE are given actually by the following complex expression:

$$\frac{d}{dt}\left(\frac{1}{2}u_i^2\right) = -\frac{\partial}{\partial x_j}\left(\frac{1}{\rho}\overline{pu_j} + \frac{1}{2}\overline{u_i^2 u_j} - 2v\overline{u_i e_{ij}}\right) - \overline{u_i u_j}\frac{\partial U_i}{\partial x_j} + \frac{g}{\rho_0}\overline{w\rho} - 2v\overline{e_{ij}e_{ij}} \tag{14}$$

In the above equation, the four components of the total changes of TKE are in the following order:

1. Transport of TKE
2. Shear Production
3. Buoyancy Production
4. Viscous Dissipation

If we take into account the fluctuating strain rate, given by the relation

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{15}$$

and replace it in (14), we get a PDE system.

3. Modeling TKE with mathematical software appliances

The equation(14) is not very easy to solve in an exact way, like most mathematical models of turbulence (Zdunkowski, 2012). Therefore, a challenging aim is to find an *exact solution* for such a PDE system. In this order, testing the modern and fast software appliances is very useful. MAPLE software has friendly and fast appliances for pde's (Abell and Braselton 2005). PDETools is a great package of tools, and we focus here on one actual and modern direction: *TW(Travelling Waves) Solutions*. The software procedure PDETools[TWSolutions] contains in fact an interesting computational process. The steps are as follows.

1. Transform the pde system into a nonlinear ode system by introducing a new variable τ following the relation

   $$\frac{\partial f_i}{\partial x_j} = C_j(1-\tau^2)\left(\frac{\partial f_i}{\partial \tau}\right) \tag{16}$$

   The resulting ODE system, polynomial in $f_i(\tau)$, and its derivatives, has all the coefficients polynomial in τ and the unknowns C_j.
2. Search for solutions of the form $f_i = \sum_{k=0}^{n} A_i^k \tau^k$ for that ODE system. Thus, an upper bound n_i for each unknown f_i is computed.
3. The complete finite expansion for each f_i, containing the unknowns $A_{i,k}$ is introduced in the ODE system obtained in step 1, and, by taking coefficients of different powers of τ, a new algebraic nonlinear system for the expansion coefficients $\{A_{i,k}C_j\}$ is built. Thus, a Travelling Wave Solution is calculated as power series expansion in tanh.
4. An elimination process splitting into cases is run through the procedure *PDEtools[casesplit]* ,which in turn uses the procedure *DEToolsRif* by default, or *DifferentialAlgebra*.
5. By default, constant solutions that are *redundant* are removed

4. Conclusions

The TW[Solutions] package is efficient in approaching and modeling the boundary layer mathematical modes because of the algorithms involved in its procedure. But, the algorithms are very calculating. Therefore, an alternating approach could be another MAPLE package, *pdsolve[system]*. This software package contains also calculating techniques, but they are differential algebra techniques and therefore there are some advantages that is useful to take into account, since the procedure is slightly easier to approach (Abell, 2005). The solving process has the steps as follows.

1 The system is first uncoupled by using *differential algebra techniques* for polynomial systems. When the PDE system, rational in the unknowns and their derivatives, contains non-polynomial coefficients, the *uncoupling* is performed by rewriting the system in polynomial form by using a differential extension approach. Due to the intrinsic nature of the differential algebra elimination process, this first step always produces (possibly many) *PDE subsystems*, such that:
   (a) The equations inside each subsystem *satisfy all the integrability conditions*
   (b) The union of the non-singular solutions of each subsystem is equal to the general and singular solutions of the original system
   (c) Provided that the original system is not subdetermined, *one of the PDE subsystems depends on a single unknown*

2 The PDE subsystem for a single unknown is solved, and the unknown removed from all other subsystems. Due to nature of the differential elimination process, after removing this single unknown, *there exists a PDE subsystem that depends on a single unknown*. Step 2 above is repeated until all the PDE subsystems obtained in step 1 are solved, thus arriving at the solution to the original input PDE system. When solving each of these PDE subsystems involving a single unknown, two situations may arise: the subsystem consists of *only one PDE*, or it consists of *many PDEs*. In the first case *pdsolve* solves the problem by using older subroutines. In "many pdes" case *pdsolve* uses a set of routines that, at each step, change variables introducing *differential invariants as new variables*.

This approach permits solving the problem when the PDE subsystem is essentially nonlinear. This makes the *pdsolve* package extremely used in practice, and it is an additional reason for taking into account this appliance in comparison with other calculating software appliances.

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