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A two-dimensional hydrodynamic model of turbulent transfer of CO₂ and H₂O over a heterogeneous land surface

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Abstract. A two-dimensional hydrodynamic model was developed and applied to describe turbulent fluxes of CO₂ and H₂O within the atmospheric surface layer over a heterogeneous land surface featuring mosaic vegetation and complex topography. Numerical experiments were carried out with a 4.5-km profile that crosses a hilly region in the central part of European Russia, with the diverse land-use patterns (bare soil, crop areas, grasslands, and forests). The results showed very strong variability of the vertical and horizontal turbulent CO₂ and H₂O fluxes. The standard deviations of the vertical fluxes were estimated for separate profile sections with uniform vegetation cover for daylight conditions in summer, and they were comparable with the mean vertical fluxes for corresponding sections. The highest horizontal turbulent fluxes occurred at the boundaries between different plant communities and at irregularities in surface profile. In some cases, these fluxes reached 10-20% of the absolute values of the mean vertical fluxes for corresponding profile sections. Significant errors in estimating the local and integrated fluxes e.g. when using the eddy covariance technique, can result from ignoring the surface topography, even in the case of relatively large plots with uniform vegetation cover.

1. Introduction
An accurate estimation of turbulent fluxes between heterogeneous land surfaces and the atmosphere is very important scientific task in numerous experimental and modeling studies [1-5]. Modern systems for monitoring greenhouse gas exchange involve a large number of field stations that provide continuous flux measurements in different types of ecosystems and geographical regions. The advantage of such monitoring systems is the use of a unified measuring technique based on the eddy covariance method, which includes a joint system for data analysis and post processing [6-7]. For flux measurements, the method ultimately requires a large and uniform land surface in the upwind direction. Surface heterogeneity may obviously lead to uncertainties in flux estimation, which can result in anomalously high or low values of H₂O and CO₂ fluxes in some cases.

The primary goal of this study is to describe the influence of vegetation heterogeneity and surface topography on CO₂ and H₂O fluxes within the atmospheric surface layer. One of the main objectives are to develop a two-dimensional (2D) model that can describe the turbulent exchange over a non-uniform land surface with complex topography and mosaic vegetation under different thermal stratification of the atmospheric boundary layer (neutral, unstable). Another objective is to quantify the contribution of horizontal advection to the ecosystem’s total CO₂ and H₂O exchange as a function of topography and key vegetation properties. A modeling experiment was conducted for a 4.5-km-long...
profile that crosses a territory with hilly topography and mosaic vegetation in the central part of European Russia.

2. Model description
The developed model is based on solving a system of averaged Navier-Stokes and continuity equations for the wind-speed-averaged components \( \mathbf{\bar{V}} = \{ \mathbf{V}_1, \mathbf{V}_2 \} \), where \( \mathbf{V}_1 \) is the horizontal component, and \( \mathbf{V}_2 \) is the vertical component of the average wind speed) using a 1.5-order closure scheme [8-9]:

\[
\frac{\partial \mathbf{V}_i}{\partial t} + (\mathbf{\bar{V}}, \nabla) \mathbf{V}_i = -\frac{1}{\rho_0} \frac{\partial}{\partial x_i} \Delta P - \sum_{j=1}^{2} \frac{\partial}{\partial x_j} \left[ \frac{2}{3} \delta_{ij} \bar{e} - K \left( \frac{\partial \mathbf{V}_i}{\partial x_j} + \frac{\partial \mathbf{V}_j}{\partial x_i} \right) \right] + \frac{\partial T}{\partial x_i} \delta_{ij} + F_i, \quad i = 1, 2,
\]

\[ \text{div} \mathbf{\bar{V}} = 0, \quad \bar{F} = -c_d \cdot \text{LAD} \cdot |\mathbf{\bar{V}}| \cdot \mathbf{\bar{V}}. \]

\( x_1 \) and \( x_2 \) are the horizontal and vertical coordinates, respectively, \( \rho_0 \) is the density of dry air (which is assumed to be constant in this approximation), \( \Delta P \) is the deviation of the mean air pressure from the hydrostatic distribution, and \( \bar{e} \) is the turbulent kinetic energy (TKE):

\[ \bar{e} = \frac{1}{2} \sum_{j=1}^{3} \langle (v'_j)^2 \rangle, \]

where the symbol \( \langle \cdot \rangle \) denotes the average over a certain time interval and space volume, \( v'_j \) is a fluctuating part of the wind speed components \( (v_j = V_j + v'_j) \), \( g \) is the free fall acceleration, \( T \) is the temperature of air, \( \delta T_v \) is the deviation of the virtual temperature \( \Theta = T \cdot (1 + 0.61q) \) from the adiabatic temperature \( T_0 \) for dry air \( (\delta T_v = T \cdot (1 + 0.61q) - T_0(x_2)) \), \( q \) is the specific humidity, \( T_0(x_2) = T_{\text{ref}} + (h_{\text{ref}} - x_2) \gamma_a \), \( T_{\text{ref}} \) is the given temperature at a certain height \( h_{\text{ref}} \), \( \gamma_a = g / c_p \), \( c_p \) is the specific heat of air at constant atmospheric pressure, \( \delta_{ij} \) is the Kronecker symbol \( (\delta_{ij} = 1 \text{ and } \delta_{ij} = 0, \quad i \neq j) \), \( F_i \) is a component of the viscous drag force induced by the presence of vegetation, \( \text{LAD} \) is the leaf area density and \( c_d \) is the drag coefficient.

The 1.5-order closure scheme assumes that the turbulent fluxes \( \langle v'_j v'_i \rangle \) can be expressed using the TKE and space derivatives of the averaged wind speed components:

\[ \langle v'_j v'_i \rangle = \frac{2}{3} \delta_{ij} \bar{e} - K \left( \frac{\partial \mathbf{V}_i}{\partial x_j} + \frac{\partial \mathbf{V}_j}{\partial x_i} \right), \]

where \( K = C_\rho \bar{e}^2 \bar{e}^{-1} \), which represents the turbulent exchange coefficient for momentum, where \( \bar{e} \) is the dissipation rate for TKE and \( C_\rho \) is the dimensionless model constant (we used \( C_\rho = 0.09 \)).

The turbulent kinetic energy \( \bar{e} \) and the rate of its dissipation \( \bar{\varepsilon} \) can be found by solving the following equations [5, 11-15]:

\[ \frac{\partial \bar{e}}{\partial t} + (\mathbf{\bar{V}}, \nabla) \bar{e} = \text{div}(K_\bar{e} \nabla \bar{e}) + P_\varepsilon - \bar{\varepsilon} - g \frac{K_T}{T_0} \frac{\partial}{\partial x_2} \delta T_v, \quad P_\varepsilon = -\sum_{i=1}^{2} \sum_{j=1}^{2} \langle v'_i v'_j \rangle \frac{\partial \mathbf{V}_i}{\partial x_j}, \]

\[ \frac{\partial \varphi}{\partial t} + (\mathbf{\bar{V}}, \nabla) \varphi = \text{div}(K_\varphi \nabla \varphi) + \frac{\varphi}{\bar{e}} \left( C_{\varphi 0} P_\varepsilon - C_{\varphi 2} \bar{\varepsilon} - C_{\varphi 3} g \frac{K_T}{T_0} \frac{\partial}{\partial x_2} \delta T_v \right) + \Delta_\varphi, \quad \varphi = \frac{\bar{\varepsilon}}{\bar{e}} \]

\[ \Delta_\varphi = 12 \sqrt{C_\mu} \left( C_{\varphi 2} - C_{\varphi 1} \right) k_\varphi \text{LAD} |\mathbf{\bar{V}}| \varphi, \]
where $K_e = K \sigma_e^{-1}$, $K_T = \alpha_a K_T$, and $K_\phi = K \sigma_\phi^{-1}$, which represent the turbulent exchange coefficients for TKE, temperature $T$, and function $\phi$, respectively. $\sigma_e$ and $\sigma_\phi$ are the Prandtl number and turbulence Schmidt number, and $\alpha_a$ is the inverse of the Prandtl number for the temperature [14-15]:

$$\alpha_a = \begin{cases} 1.35(1+13.5 Ri)^{-1}, & Ri \geq 0, \\ 1.35(1-15 Ri)^{1/4}, & Ri < 0, \end{cases}$$

$$Ri = \frac{g}{T} \sum_{i=1}^{2} \frac{\partial T}{\partial x_i} + \frac{\partial T}{\partial x_i} + \frac{1}{\rho_0 c_p} \left( \frac{\partial T}{\partial x_i} + \frac{1}{\rho_0 c_p} \right).$$

$Ri$ is the Richardson number, while $C_{\phi 1}$, $C_{\phi 2}$, and $C_{\phi 3}$ are model constants [10, 14-15].

The main system of equations also includes diffusion and advection equations for turbulent transfer of sensible heat, CO$_2$ ($C_s$) and specific humidity ($q$) at the interface between the soil, vegetation, and atmosphere [5]:

$$\frac{\partial T}{\partial t} + (\mathbf{V}, \nabla)T + T \cdot \mathbf{V} = \text{div}(K_T \cdot \nabla T) + \frac{T}{T_0} \cdot \mathbf{V} - \frac{1}{\rho_0 c_p} \left( \mathbf{V} + \nabla T \right) + \frac{1}{\rho_0 c_p},$$

$$\frac{\partial C_s}{\partial t} + (\mathbf{V}, \nabla)C_s = \text{div}(K_C \cdot \nabla C_s) + F_C, \quad \frac{\partial q}{\partial t} + (\mathbf{V}, \nabla)q = \text{div}(K_v \cdot \nabla q) + \frac{E}{\rho}.$$
\[ \lambda E = \frac{\Delta(T_g) \cdot R_{soil} + \rho c_p (e_a(T_g) - e_a) \cdot T_g}{\Delta(T_g) + \gamma_p} \cdot w, \]

where \( \Delta(T_g) \) is the rate of change of saturation water pressure at a particular air temperature, \( R_{soil} \) is the soil radiation balance, \( g_a \) is the exchange coefficient for H$_2$O and \( w \) is the soil moisture.

We next describe the photosynthesis of the plant canopy and respiration rates. This was accomplished using an aggregated approach based on a model by Ball et al. [17] using Leuning’s modification [18], the Beer-Lambert equation for solar radiation penetration within a plant canopy [19], and an algorithm describing the leaves’ stomatal conductance response \( g_s \) to incoming photosynthetic active radiation (PAR) [20]:

\[ F_c = -\frac{LAD}{a_1} (g_s - g_0)(C_s - \Gamma_s) \left( 1 + \frac{D_s}{D_0} \right), \quad g_s = g_{max} f(PAR), \quad f(PAR) = 1 - \exp(-\beta_s \cdot PAR), \]

where \( g_0 \) is the value of \( g_s \) at the light compensation point, \( \Gamma_s \) is the CO$_2$ compensation point, \( D_s \) is the dimensionless water vapor partial pressure deficit at the leaf surface, and \( a_1 \) and \( D_0 \) are empirical coefficients. The PAR profile within the plant canopy is described as:

\[ PAR(x_2) = PAR_{hc} \cdot \exp \left( -k \int_{x_2}^{hc} LAD(z)dz \right), \]

where \( PAR_{hc} \) is the value of PAR at the canopy height \( hc \), and \( k \) is the extinction coefficient.

The soil CO$_2$ emission is considered as a function of the soil temperature and moisture. It is also assumed that the soil CO$_2$ emission rate is dependent on the wind speed and turbulence intensity at the ground surface layer.

3. Modeling experiments

Figure 1 shows the 4.5-km profile used to quantify the influence of surface topography and vegetation heterogeneity on the turbulent CO$_2$ and H$_2$O fluxes. The vegetation along the profile is represented by a mosaic of bare soil, agricultural crops, and small woody areas. The vertical and horizontal turbulent fluxes of CO$_2$ and H$_2$O were calculated for three main model scenarios. The first one considers the actual surface topography and vegetation heterogeneity with the assumption of neutral thermal stratification of the atmospheric surface layer. The second one considers the vegetation heterogeneity but ignores the surface topography. Neutral atmospheric stratification is also assumed in this scenario. In the third scenario, the ecosystem fluxes are calculated for the actual vegetation heterogeneity and surface topography under unstable atmospheric stratification due to the ground surface and vegetation overheating. All numerical experiments were conducted for different wind directions.

![Figure 1](image-url)
Figure 2. Modeled vertical turbulent CO$_2$ fluxes at 30 m above a ground surface calculated for different scenarios assuming: a) neutral atmospheric conditions, while ignoring the surface topography; b) neutral atmospheric conditions with the real surface topography; and c) unstable atmospheric conditions with the real surface topography. d) Comparison of fluxes calculated for different model scenarios. The blue line shows the difference between fluxes for the scenarios 1 (b) and 2 (a); the violet line shows the difference between fluxes for the scenarios 1 (b) and 3 (c).

Figure 3. Modeled vertical LE fluxes along the selected profile at 30 m (blue line) and 50 m (dotted violet line) above a ground surface calculated for different scenarios assuming: a) neutral atmospheric conditions with the real surface topography; b) neutral conditions while ignoring the surface topography; and c) unstable conditions with the real surface topography. Comparison of fluxes between different model scenarios: d) difference between fluxes for the scenarios 1 (a) and 2 (b); e) difference between fluxes for the scenarios 1 (a) and 3 (c).
4. Results and discussion

The results of the modeling experiments showed that the complex topography and mosaic vegetation cover have a significant influence on the atmospheric CO$_2$ and H$_2$O fluxes (figures 2-5). The greatest flux disturbances occurred at the boundaries between different plant communities, especially at windward forest edges and in the profile sections with uniform vegetation cover but with some irregularities in the surface topography (e.g., hilltops, hollows). In particular, uniform forest plots are characterized by significant horizontal heterogeneity of vertical fluxes (figures 2-3) and permanent non-zero horizontal fluxes (figures 4-5), despite the relatively large size of the plots (>500-600 m).

The variability of both the vertical and horizontal fluxes is minimal for scenarios in which the surface topography is ignored (horizontality of the ground surface is suggested). The highest variability occurs in scenarios that assume the real complex topography and unstable thermal stratification of the atmospheric boundary layer. The highest horizontal turbulent fluxes occur at the forest edges, in some cases reaching 10-20% of the absolute values of the mean vertical fluxes for the corresponding forest plot. The standard deviation of the vertical fluxes decreases as the height above the ground surface increases (figure 3).

The flux pattern over agricultural crops is mainly influenced by downwind surface properties. In the case of upwind from the bare soil area, the spatial pattern of vertical fluxes over agricultural crops is relatively uniform, and the horizontal fluxes for all model scenarios vary around zero. In the case of upwind from some forest patches, the air flow disturbances are manifested at a rather long distance from the leeward forest edge (up to 400-500 m), and the steady-state air flow is not achieved, even with model assumptions suggesting a flat topography (scenario 1). There is quite insignificant change in the vertical CO$_2$ and H$_2$O fluxes with the height over agricultural fields and bare soil, in contrast to forest sites.
There was very high heterogeneity of atmospheric fluxes in the numerical experiments. This illustrates a great difficulty in finding the optimal position for flux measuring stations for areas with mosaic vegetation structure, even in the case of flat topography. Modern post processing techniques for eddy covariance data use footprint analysis to describe the upwind area where the atmospheric flux measured by instruments is generated [1]. The flux footprint functions estimate the location and relative importance of passive scalar sources that influence flux measurements at a given height of a measuring device. The results are dependent on the device height, atmospheric stability, and surface roughness [21]. Several studies describe the possible effects of surface topography on atmospheric fluxes by estimating the vertical and horizontal advection terms [4]. Further investigation is required to estimate the effects on atmospheric fluxes of the air flow disturbances that arise at the boundaries between different types of vegetation and at topographic irregularities situated at some distance from the measuring systems. Such efforts will require accurate consideration to obtain representative fluxes.

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