ESTIMATION THE HEIGHT OF OZONE FORMATION IN THE ATMOSPHERIC BOUNDARY LAYER

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ABSTRACT

Calculation results with algorithm reconstitution of vertical ozone source profile, shows that in inside daily period, in background areas of West Siberia, photo-chemical ozone formation prevailing above ozone inflow process from overlying stratum.

Keywords: ozone, vertical source profile ozone, vertical concentration distribution ozone

1. INTRODUCTION

Ozone plays primary role in photo-chemical processes occurring in atmosphere boundary layer. Ozone is the fourth in importance green gas. In addition, it is make bad influence on the vegetation and human health. In boundary layer there are two main ozone sources, first advection transfer from overlying stratum; second photo-chemical generation from precursor gases directly inside boundary layer. In present time, the balance of this sources still unknown. In this work, we made reconstitution of vertical ozone source profile by solving the inverse problem for the specific measurement day. As main parameters for the solving inverse problem was taken results from airborne vertical ozone distribution sensing in boundary layer.

2. MEASUREMENT DATA AND CALCULATION METHODS

For the calculation were used the results from airborne and aerologic sensing held August 8, 2013. Measurements carried in the background area of the Tomsk region, over the green gasses monitoring post near the Berezarechka village ($56^{0}08'$ N, $84^{0}20'$). Over experiment area, there was northeastern part of the cyclone and partly cloudy. Speed of wind was 2.5 meters/second. Detailed measuring complex description based on An-2 aircraft showed in work [2].

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Let us formulate inverse problem. Introduce rectangular dimensionally-temporal area $(z,t) \in \Omega_T := [0,Z] \times [0,T] \in \Re^2$. In this dimension, consider transport model of chemicals substance in the atmosphere:

$$\frac{\partial\varphi}{\partial t} + w\frac{\partial\varphi}{\partial z} = \frac{\partial}{\partial t}\mu\frac{\partial\varphi}{\partial z} + f(z,t) \in \Omega_T$$
(1)

$$-\mu \frac{\partial \varphi}{\partial z} + \beta_L \varphi = \alpha_L, \ x = 0, \tag{2}$$

$$\mu \frac{\partial \varphi}{\partial z} + \beta_R \varphi = \alpha_R, \ z = H, \tag{3}$$

$$\varphi = \varphi_0, \ t = 0. \tag{4}$$

where $\varphi(z, 0)$ is condition function, describing chemical substance concentration field, w(z, t) - vertical transfer speed, $\mu(z, t)$ - diffusion coefficient, $\alpha_L(t), \alpha_R(t)$ - apriori source meanings from the edge of the area, β_L, β_R specified constants, f(z, t) - volume source function.

Direct problem is to determine from (1)-(4) by known. As far as we have M vertical distribution concentration substance (ozone) profiles I_m , obtained during the airborne sensing, so we can make:

$$\varphi(z, t_m) = I_m(z), z \in [0, Z], t_0 = 0, t_m \in [0, T], m = 0, 1, \dots M - 1$$
(5)

Inverse problem is to obtain f from (1)-(5) by known $I, \alpha_L(t), \alpha_R(t), \mu, w$. Assuming that $\varphi^0(z) = I_0(z), z \in [0 < Z]$. For estimating f, we will use optimization solutions method [1] of inverse problem and minimize target functional by gradient algorithm.

$$J_a(f) = \sum_{m=1}^{M} \|\varphi(z, t_m) - I_m\|^2 + \alpha \|Uf\|^2$$
(6)

On condition that φ and f connected by model (1)-(4). Using Euler-Lagrange principle, we can receive that gradient (6) is:

$$\nabla J_a = \psi(z,t) + 2\alpha (U^* U f)(z,t) \tag{7}$$

Where ψ is decision of conjugated equation.

$$-\frac{\partial\psi}{\partial t} - w\frac{\partial\psi}{\partial z} = \frac{\partial}{\partial t}\mu\frac{\partial\psi}{\partial z} + +2\sum_{m=1}^{M}(\varphi(z,t_m) - I_m(z))\delta(t-t_m), (z,t) \in \omega_T$$
(8)

$$-\mu \frac{\partial \psi}{\partial z} + \beta_L \psi = 0, z = 0, t \in [0, T]$$
(9)

$$\mu \frac{\partial \psi}{\partial z} + \beta_R \psi = 0, z = Z, t \in [0, T]$$
(10)

$$\varphi(z,0) = \varphi^0(z), z \in [0,Z] \tag{11}$$

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As operator, U we will consider time derivative for the source smoothness

$$U\varphi = \frac{\partial\varphi}{\partial t} \tag{12}$$

Conjugated gradient method used for the minimization target functional (6). For inverse problem solving, $\mu(z,t)$ coefficient turbulence diffusion calculated by results of the ground heat flow measurements and friction tension, and by vertical and wind profiles based on k-theory. Vertical speed w in formulas (1)-(3) and (8)-(10) was set as constant -1 cm/s (minus specify the downward direction of speed). The precipitation rate of impurities, in our case, was taken constantly 0.6 cm/s.

To test the algorithm used by a source in the form of Gaussian function(13) (Fig. 1):

$$f(t,z) = \frac{A_T A_Z}{2\pi\sigma_T \sigma_Z} e^{-(\frac{(t-t_0)^2}{2\sigma_T^2} + \frac{(z-z_0)^2}{2\sigma_z^2})}$$
(13)

where, $A_T = 0.3$ h, $\sigma_T = 2$ h, $t_0 = 15$ h, $A_z = 125$ m, $\sigma_z = 50$ m, $Z_0 = 300$ m.



Figure 1. Altitude-time distribution power source modeled (13) a), recovered b).

3. RESULTS

Figure 2a, shows vertical concentration and reconstitution ozone power source profiles (fig. 2b). We can see that power source profile has two extremes with maximum in boundary layer and minimum in upper part of boundary layer at the engagement zone. Height and quantity of maximum ozone source depends on a time of the day. In morning time at 8:00 and 11:30, source power is nearly constant in whole boundary layer. At 15:00 and 19:30, maximum highlighted at altitudes from 300 to 600 meters. Average power capacity of ozone source in boundary layer was 0.3 nmol/m³s, and the source located above boundary layer was 0.0012 nmol/m³s, that is indicates effluent predominance in the stratum above boundary layer.



Figure 2. Vertical ozon distribution profiles a), altitude-time distribution power source ozone recovered b) on 8.08.2013.

4. CONCLUSION

Calculation results using reconstitution algorithm of vertical ozone source profile, shows that photochemical ozone formation process in boundary layer, predominate over processes in overlying stratum, inside daily scale in the background area of West Siberia.

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