A new approach to estimating of the power of nitrogen oxides emissions from the anthropogenic source

N Tikhonov¹, S Zakharova¹ and M Davydova¹
¹Lomosov Moscow State University, Moscow, Russia
E-mail: niktandr@yandex.ru, sa.zakharova@physics.msu.ru, m.davydova@physics.msu.ru

Abstract. The paper presents a new approach to estimating of the power of nitrogen oxides emissions from the anthropogenic source. Authors created the model that describes the dynamics of the formation of a plume from the point anthropogenic source, coordinated in the complexity with the amount of the available data. Based on the proposed model, it is become possible to estimate the emission power by the satellite photographs obtained from the Resource-P series satellite. This estimate is the particular interest in the controlling emissions, which is the complex and non-trivial problem. Also authors determined the distribution of the height-integral amount of nitrogen dioxide over the Hebei Province, China, and compared it with the experimental data. The obtained estimates of the emission power can be used to integrate it into the complex chemical transport models.

1. Introduction
Nowadays there is a large number of the industrial enterprises in all developed countries. These enterprises release a large amount of the substances such as CO, NO, NO₂, the aerosols and the volatile organic compounds into the atmosphere. The increased concentration of these compounds leads to the extreme environmental situations. Nitrogen oxides are formed during the combustion of the fuel at the thermal power plants, the metallurgy and other areas of the industrial production. Also, the appearance of the nitrogen oxides is influenced by the exhaust gases. The minimal consequences of these emissions are the eye and nasopharyngeal irritation and the shortness of the breath. Another example of these effects is the photochemical smog. It is the aerosol that occurs when exposed to sunlight on the nitrogen oxides, the hydrocarbons and volatile organic compounds. In consequences, there is a need for the predicting of the spread of that kind of substances, accounting of the emissions from the enterprises and controlling them. Currently, there are various numerical chemical transport models such as HYSPLIT, SILAM, etc. The simulation results often do not agree with the measurements taken, for example, at the atmospheric monitoring stations [1]. The discrepancies are explained by the lack of the qualitative information on the spatiotemporal structure of the distribution of emissions of the anthropogenic gas and aerosol impurities [2, 3]. Thus, it is necessary to know the emission power in order to correctly set the emissions in such models. The following information was available to determine the emission power:
• the integrated NO\textsubscript{2} storage with the high spatial resolution at a certain point in the time \cite{4, 5};
• the direction and average wind speed for the period of the time during which there was the transfer of pollution from the ejection point to the boundary of the area \cite{6};
• the background levels of NO and NO\textsubscript{2} gases in the atmosphere \cite{7};
• the coefficient of the turbulent diffusion \cite{8}.

2. Construction of the model

The environmental problems are usually distinguished by a large number of operating factors and a small amount of experimental data. Therefore, it is very important to create the model that is adequately consistent with the amount of experimental data. The model should take into account the main factors that influence on the behavior of the quantity in question, but at the same time contain a number of the parameters that can be determined from the available experimental data.

As the variable we consider the total distribution of the integral storage of NO\textsubscript{2} and NO, counted from the background level. We divide the region in accordance with Fig.1, where \(x\) is the axis in the direction of wind speed, \(y\) is in the perpendicular direction, parallel to the surface of the Earth. When \(t > 0\), \(u\) is the solution of the problem:

\[
\begin{align*}
  a \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} &= a^2 \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + f_0 \delta(x) \delta(y), \quad t > 0 \\
  u(x, y, 0) &= 0, \quad u \to 0, \text{ when moving away from (0,0)}
\end{align*}
\]  

\[(1)\]

where \(f_0\) – the total emission power, \(a\) – the coefficient of the turbulent diffusion, \(v\) – the wind speed.

Figure 1. The partition scheme of the area in which the solution is sought

There is no exact solution of the problem (1). Let’s try to construct the approximate solution, neglecting the small quantities.

Let \(f_0 = Const\), \(v = Const\) and \(t > 0\) such that \(u\) is stationary (\(\partial u/\partial t = 0\)). In the region \(x < 0\), the diffusion effect balances the transport effect in this region only for large values of \(\text{grad} u\) and, accordingly, a small length of the segment \(Ob\) in Fig.1. The substance entering the region due to diffusion is transferred by the wind to the region \(x < 0\) in the form of the stream narrow by \(y\). This flow is added to the flow going directly from the pollution source to the region \(x > 0\). As a result, for \(x = 0 + 0\), the common flow is created with the density of \(F(y)\) and the total power of \(f_0\). The above considerations suggest that the dependence \(F(y)\) should have the form of the peak smeared out due to the diffusion process in the region \(x < 0\), from where the part of the substance arrives.
2.1. Approximate solution in the region \( x > 0 \)

In the region \( x > 0 \) (Fig. 1), the transport of the matter along the axis \( x \) predominates (gradu is relatively small). Then in this region \( u(x, y) \) is the solution of the following problem:

\[
\frac{\partial u}{\partial x} = a^2 \frac{\partial^2 u}{\partial y^2}, \quad u(0, y) = \frac{F(y)}{v}.
\]  

Given the above, we choose the function \( F(y) \) in the form:

\[
F(y) = \frac{f_0}{2a\sqrt{\pi\tau_0}} e^{-\frac{y^2}{4a^2\tau_0}}.
\]

With this choice, \( F(y) \) has the required form and the following holds:

\[
\int_{-\infty}^{\infty} F(y) dy = f_0.
\]

The value of the parameter \( \tau_0 \) – characterizes the degree of smearing of the flow of matter entering the region \( x > 0 \). This value will be determined below. The solution of the problem (2) in the region \( x > 0 \) has the form:

\[
u(x, y) = \frac{f_0}{\sqrt{2\pi(\tau + \tau_0)}} e^{-\frac{y^2}{4(\tau + \tau_0)}} , \quad \tau = x/v.
\]  

2.2. Approximate solution in the region \( x < 0 \)

Let’s say that \( U(x) = \int_{-\infty}^{\infty} u(x, y) dy \). Then from (1), taking into account that \( \partial u/\partial t = 0 \), we find:

\[
u \frac{\partial U}{\partial x} = a^2 \frac{\partial^2 U}{\partial x^2} , \quad U|_{x=0} = \frac{f_0}{v}.
\]

The solution of the problem (4) can be represented as:

\[
U(x) = \frac{f_0}{v} \left( 2 - e^{-\frac{x}{\tau}} \right)
\]

Let’s keep the same dependence from \( x \) for \( u(x, y) \) at \( x < 0 \). Then in this region we have:

\[
u(x, y) = \frac{f_0}{\sqrt{2\pi(\tau + \tau_0)}} e^{-\frac{y^2}{4(\tau + \tau_0)}} \left( 2 - e^{-\frac{x}{\tau}} \right) , \quad x < -\frac{a^2}{v} \ln 2 , \quad x < 0,
\]

The solution (6) satisfies the condition (5) and is conjugated by the value of \( u \) to the solution (3) at the point \( x = 0 \).

2.3. \( \tau_0 \) determining

The parameter \( \tau_0 \) characterizes the width of the flow of matter passing from the region \( x < 0 \) to the region \( x > 0 \). Let’s consider the small level \( u = u_{\text{max}} e^{-\lambda} \), where \( u_{\text{max}} = u(0, 0) \) and the point \( b \) (Fig.1), corresponding to the intersection of this level with the line \( x = 0 \). Let’s suppose that at point \( b \) the influx of the matter due to diffusion of \( a^2 u_{yy} \) is completely balanced by the transfer of \( vu_x \). Then at the point \( b \) we get:

\[-vu_x = a^2 u_{yy},
\]

thus \( \tau_0 = \left( \lambda - \frac{1}{2} \right) \left( \frac{a}{\tau} \right)^2 \). It was verified that changing the value of the small parameter \( \tau_0 \) has little effect on the form of \( u \) for the values of \( x > \tau_0 v \). Therefore, let’s say \( \tau_0 = \frac{1}{2} \left( \frac{a}{\tau} \right)^2 \), which corresponds to \( \lambda = 1 \).
Note
The solution $u$ will be obtained in the form of time-dependent relations. For $x > 0$ we introduce the delay time $\theta$ in accordance with the equality:
\[ x = \int_0^\theta v(t)dt. \] (7)

Then the equality (3) takes the form:
\[ u(x, y) = \frac{f_0}{v(t-\theta)2a\sqrt{\pi(\theta+\tau_0)}} e^{-\frac{x^2}{4a^2(\theta+\tau_0)}}, \quad x > 0. \] (8)

For $x < 0$, taking into account the small size of the diffusion region (shaded by the frequent lines in Fig.1), in expression (6) let’s set $v = v(t)$.

2.4. Determination of the distribution of nitrogen dioxide integral storage
The anthropogenic source emits the nitric oxide (NO) into the atmosphere. The emitted nitric oxide is converted into NO$_2$ as a result of the chemical reactions, whose integral storage has been recorded. Let’s denote the total amount of NO$_2$ in the vertical column of air counted from the background level as $c(x, y, t)$. The transition of NO to NO$_2$ occurs in a rather complicated way [9]. The speed of reactions depends on many external factors. It is impossible to establish this dependence due to the small number of measurements. Therefore, the simplest description of the changes in the value of $c$ in the case of a constant wind speed seems most justified in this situation:
\[ \frac{\partial c}{\partial \tau} = \beta (u - c) - \gamma c, \quad c|_{\tau=0} = 0 \] (9)

where $\beta$ is the effective kinetic parameter characterizing the rate of the transition of pollution from the total form (NO + NO$_2$) to the NO$_2$ form, and $\gamma$ – characterizes the rate of NO$_2$ decay. Note: in the case of variable wind speed in (9) it is necessary to use the local time $\theta$ defined in (7).

Thus, the process model consists of the set of equations (5), (6), (7) and (9).

3. Estimating of the emission power
Let’s use the formulated model to estimate of the power of anthropogenic pollution source of one of the enterprises located on the Hebei Province, China. The picture taken on the September 29, 2016 at 4:30 UTC is available for this area. In order to estimate of the emission power, it is necessary to determine the parameters of the model: $\gamma$ and $\beta$.

3.1. Determining of the coefficient $\gamma$
The value of the coefficient similar to $\gamma$ can be taken from [9]. In this paper, the effective value of $\gamma$ was found. To verify the accordance of the taken value, the numerical experiments were carried out. In these experiments the model solution with different $\gamma$ values was compared with the experimental data. The numerical experiments have shown that for $\gamma \in [0, 8 \cdot 10^{-5}]s^{-1}$, the solution does not change much (Fig.2), and with the available data quantity it is not possible to select a specific value. Thus, within this model, it is advisable to use the value $\gamma = 1.4 \cdot 10^{-5}s^{-1}$ from [9].
Figure 2. Dependence of the difference of model solution and the experimental data on $\gamma$

Figure 3. Comparison of the experimental data and the model solutions for the determining parameter $\beta$ (region 1)

3.2. Determining of the coefficient $\beta$

We can estimate the value of $\beta$ by the rate at which the observed concentration $c$ near the pollution source in the region 1 increases from the zero to the maximum (Fig.3). The dependence of $c$ on $x$ for $y = 0$ in the region $x < 0$ is described by the equation:

$$ v \frac{\partial c}{\partial x} = \beta (u(x,0) - c) - \gamma c, \quad c|_{x=-\frac{x_0^2}{v} \ln 2} = 0, \tag{10} $$

where $u(x,0)$ is defined in (6). The constant $\beta$ is found by the minimizing of the squared difference of the solution of the problem (10) and the experimental data.

In Fig.3 the solid line is the solution of the problem (10), the points are experimental data. Region 2 corresponds to a sharp change in the magnitude of the wind speed.
3.3. Estimating of the emission power

The estimate of the emission power $f_0$ was determined by the minimizing of the squared difference of the model solution and the experimental data over the entire definition region. To find $f_0 = \text{Argmin} ||u_{\text{model}} - u_{\text{exp}}||^2$, we used the scipy module for python3. As a result, we obtained $f_0 = 5775 \cdot 10^{15} \text{mol} \cdot \text{cm}^{-2} \text{s}^{-1}$.

3.4. Comparison with the experimental data

In the Fig.4 compares the model solution with selected parameters $\gamma$, $\beta$, $f_0$ with the experimental data in the section by the plane $y = 0$. The Fig.5a shows the level lines of the integral storage of nitrogen dioxide obtained by the model, the Fig. 5b shows the experimental data. The Fig.6(a-c) shows the dynamics of the formation of a plume of nitrogen dioxide integral storage.

4. Conclusions

Using the presented model, it is possible without the significant computational costs:
estimate the power of emissions from the anthropogenic pollution source from a single orbital image (such estimates can be suitable both for the monitoring and for the further use in the more complex chemical transport models);

- make a short-term distribution forecast (a long-term forecast is impossible due to the variability of $\beta$, $\gamma$);

- set the dependencies of $\beta$, $\gamma$ on the various factors (the lighting, the humidity, etc.) if there is enough the data. For example, the similar pictures but for the different time moments;

- construct a test example for the checking of the quality of calculations for the more complex models (as an extreme case).

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