Physical and mathematical modeling of pollutant emissions when burning peat

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Abstract. The article presents an original neural network model of CO dispersion around the experimentally simulated peat fire. It is a self-learning model considering both the measured CO concentrations in the smoke cloud and the refined coefficients of the main equation. The method is recommended for the development of air quality control and forecasting systems.

1. Introduction

Peat deposits are found in many places, but the world's largest peatlands are the West Siberian Lowland, the Hudson Bay Lowland, and the Mackenzie River Valley [1]. Indonesia is known to have the largest tropical peatlands than any other country in the world [2]. The peat ecosystem is the most efficient carbon sink on the planet, for that reason, peat fires are significant sources of carbon dioxide and other greenhouse gases [3]. Peat fires produce a large amount of smoke that negatively affects air quality, public health, social activities, and the peatland ecosystem as a whole. In addition, peat fires release mercury into the atmosphere at a rate 15 times greater than upland forests, which may be a serious human health concern [4].

Peatland fires are of major concern in the Russian Federation [5-7]. The record-breaking heat wave and over 600 peatland and forest fires in the Central European part of Russia in summer 2010 resulted in a heavy smog blanketing large urban regions and caused numerous public health problems as a consequence [8].

There are two types of fires in peatlands: flaming fires and smouldering fires. The first ones occur at a temperature above 600 K and have high combustion efficiency, with more CO₂ and less smoke emitted. The second ones have higher CO and smoke emissions. Fires in peat tend to fall in the smouldering phase and persist in such a way for extended periods of time [9].

Peat can burn deep underground for meters, even in damp conditions and in winter time under the snow layer (Fig. 1). Peat fires are difficult to extinguish, and severe fires in peatlands can last for months. Winter peat fires are often smoldering fires that create a lot of smoke because of incomplete combustion and result in greater emissions of carbon monoxide and other harmful substances including PM₁₀ and PM₂.₅, VOCs, etc. [5, 9-11].

If a peat fire develops near a motorway, the smoke from the burning peat-bog reduces the visibility, makes the breathing difficult, affects the human nervous and cardiovascular systems and may finally result in traffic accidents or in an emergency.
Such an emergency, caused by a peat fire, lasted in Irkutsk Region (situated in the West Siberian Lowland) near the Federal Highway “Siberia” from 26.10.15 to 15.01.16 (Fig. 2).

Atmospheric chemical transport models are widely used for the management of air quality strategies [11-13], however the accurate temporal and spatial estimates of emissions from peat fires are problematic because of uncertainties in the size, location, quantity of fuel consumed, relative proportions of flaming versus smoldering combustion, their temporal and spatial variability [9, 12]. We have previously developed an original neural network model on the base of real experimental data of CO emissions from the peat fire happened in the Irkutsk region near the Federal Motorway P-255 “Siberia” in fall-winter 2015-2016 [14, 15]. The results of numerical investigations showed that the proposed approach could be recommended as a useful tool for the air quality management. However, the technique still needs further improving through the obtaining of more accurate primary data that can be received from the experimental simulation of the peat fire, and through the step-by-step self-learning of the neural network model.

2. Modeling technique

2.1. Experimental procedure and the results of direct CO measurements

In order to develop a correct experiment simulating real peat fire, we should clarify the mechanism of fire development. Peat is a product of incomplete decomposition of plant materials under the conditions of excess humidity and insufficient aeration [6, 7]. The structure and composition can be modeled by a porous multiphase reactive medium consisting of cellulose, lignin, water in a liquid-droplet state, condensed products of pyrolysis, ash, and a gas phase [6, 7]. Peat has a high carbon content and can burn under low moisture conditions. Once ignited by the presence of a heat source (e.g., a burning match or a cigarette), it smolders for very long periods of time. Fig. 3 shows a schematic cross-section of the combustion zone of the surface peat layers [16].
A peat fire was simulated outdoor using 25 kg of a natural peat sampled in the Leningrad Region. The sample of the peat was laid on a fireproof substrate and was burned using charcoal (Fig. 4). The peat has been smoldering in a flameless combustion mode for 40 minutes. The place of ignition was considered as zero in the measurement experiments (Fig. 5).

We used two types of gas analyzers for the measurement of CO concentrations. Testo-330-2LL suits for the determination of CO content in combustion gases, and we measured with it the concentration of carbon monoxide near the simulated peat fire. PGA-200 is equipped with a more sensitive detector, and it is designed for the determination of ambient CO concentrations. The speed of wind was measured using the anemometer ATE-1033. The wind velocity during the experiment varied within 3-5 m/s. Technical characteristics of all instruments are summarized in Table 1.

### Table 1. Technical characteristics of the measuring instruments

| Measuring instrument | Measured Parameter | Detector       | Detection limits | Accuracy   |
|----------------------|--------------------|----------------|------------------|------------|
| PGA-200 (Electrostandart, CO) | Electrochemical | 0-120 mg/m³ | ± 5 mg/m³ |
The results of the CO concentration measurements in the smoke propagation zone around the simulated peat fire at different distances from it are shown as blue points in the Fig. 5. We inputted these values as primary data when we developed the mathematical model of the pollutant diffusion in the air.

2.2. Justification of the mathematical model. Neural network approach

The equation of diffusion in the atmosphere, based on the physical law of conservation of the flow of matter. According to Berlyand [17-18], such parameters as instant concentrations of CO pulsed deviations from these values and the velocity of the CO diffusion should be taken into consideration while developing an emission model of the peat fire near the motorway. The problem is simplified by the application of the turbulent diffusion model:

$$\frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} + v \frac{\partial q}{\partial y} + w \frac{\partial q}{\partial z} = \frac{\partial}{\partial x} \left( k_x \frac{\partial q}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial q}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial q}{\partial z} \right) - \alpha q ,$$

where $q$ is the concentration of pollutant (g/m$^3$); $x$ and $y$ are the horizontal axis (m); $z$ is the vertical axis (m); $t$ is the time (s); $u$, $v$, $w$ are the components of the wind speed in the direction of the axes $x$, $y$, $z$, respectively, (m/s); $k_x$, $k_y$, $k_z$ are the components of the coefficient of turbulent diffusion along the Cartesian coordinate axes; $\alpha$ is the coefficient taking into account probable metabolism of CO in the atmosphere.

The authors of the present paper have a long-term positive experience of the application of this model for the estimation and the forecast of transport and fire-related air pollution (K-theory) [19-21]. The K-theory approach takes a long time and does not indicate inaccurate parameters of the problem, obtained from measurements. To solve these problems, we propose to apply the neural network approach.

On the base of the measurements, there was developed a neural network model with parameters (weights) tuned via optimization methods. The RProp-method and the combination of Cloud- and RProp-methods were in use [22-24]. The neural network model of the complex system can gather pieces of heterogeneous information – differential equations, conservation laws, equations of state, symmetry conditions, etc. The information exchange via neural network parameters between different levels of hierarchy makes computing less resource consuming.

Equation (1) can be greatly simplified for the solution to the problem concerning peat fire. In the steady state, we can assume that $\frac{\partial q}{\partial t} = 0$.

The $OZ$ – axis pointed upward, so, $w$ for heavy particles, having own sedimentation rate (with the sign "−"), is equal to that rate, and $w$ for light fractions is equal to 0. We also assume that the average turbulent flow of pollutants at the earth surface is small and the exchange coefficients are constant. We consider further only the light fraction and suppose that the concentration of CO satisfies the equation:

$$u \frac{\partial q}{\partial x} + v \frac{\partial q}{\partial y} - k \left( \frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} \right) = Q, \quad (x,y) \in \Omega ,$$

where $k$ is the diffusion coefficient, and $Q$ is the source term.
where \( Q \) is constant in the area of peat fire \( K \subseteq \Omega \), \( Q = 0 \) out of the fire; \( k \) is the known parameter, \( u, \ v \) are the known wind speed components corresponding to the measurements.

We can move the origin to the center of the peat fire, which we consider a superficial source of CO emission having a circular geometry.

In the second place, we orient the \( OX - \) axis in the direction of the wind by turning the coordinates. For the physical model of the "smoke geyser" we can assume that the component \( v \) of the wind speed in the direction of the \( OY - \) axis is equal to \( 0 \).

We deal further with such parameters as the radius of the area of the peat fire and the wind speed \( u \). In the first version of the program, they are fixed and determined at the beginning as other input data. They can be changed further by the program learning. We will find a solution of the equation (2) in the form of neural network model:

\[
q(x,y) = \sum_{i=1}^{N} c_i \exp \left[ -a_i (x-x_i)^2 - b_i (y-y_i)^2 \right],
\]

whose weights – parameters \( a_i, b_i, x_i, y_i \) and \( c_i \) can be found by minimizing the error functional:

\[
J = \sum_{j=1}^{M} \left[ u \frac{\partial q(\xi_j,\eta_j)}{\partial x} - \frac{\partial^2 q(\xi_j,\eta_j)}{\partial x^2} - \frac{\partial^2 q(\xi_j,\eta_j)}{\partial y^2} - Q(\xi_j,\eta_j) \right]^2,
\]

where \( \{(\xi_j,\eta_j)\}_{j=1}^{M} \) are the trial points in the area where the solution is built, they are updated every 3-5 steps of the error functional minimization; \( Q(\xi_j,\eta_j) = 1 \) in the area of the peat fire \( K \) and \( Q(\xi_j,\eta_j) = 0 \) at other points out of the area.

We transform (2) to the form

\[
\frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} = \frac{u}{k} \frac{\partial q}{\partial x} - \frac{Q}{k}.
\]

Thus, the solution to the problem is reduced to the development of an approach for determining the parameters \( V_x = \frac{u}{k} \) and \( \frac{Q}{k} \).

3. Results of mathematical neural network simulation of CO diffusion from the "smoke geyser"

We applied a three-step methodical approach to develop an adequate neural network model:

1) Construction of the neural network approximation using only the data from the experimental measurements;
2) Determination of the coefficients in the equation (2) using the approximation received at the first step;
3) Simultaneous determination of the equation coefficients and the construction of the neural network approximation using both experimental data (step 1) and the refined equation (step 2).

An appropriate computing program was developed for each step.

3.1. Step 1

Step 1 deals with the neural network approximation built on the base of experimental measurements. Fig. 6 shows the neural network approximation of CO dispersion at the height of human respiration (1.5 m) in the entire area of the smoke propagation.
3.2. Step 2
The results of Step 1 allowed us to determine the coefficients in the equation (2) or (5) and find the neural network solutions for the CO dispersion right above the smoldering source. We used random initial values of the coefficients in the equation (5). Fig. 7 demonstrates the neural network solution of the stationary process of CO diffusion directly above the burning source.

3.3. Step 3
Step 3 supposes implication of heterogeneous information, namely, the results of the real measurements from the Step 1 and the equation coefficients from Step 2, in order to find the neural network solution and to refine the coefficients of the equation (5).

The results of calculation were unstable for the random initial coefficients of the equation. In order to overcome this problem, we determined the coefficients of the equation (5) by a linear regression.
performed on the base of 20,000 random points through the substitution in the equation of the trial function realized in the Step 1 computing program. Such an approach allowed us to find fixed values of the coefficients: \( Q = 1741.88 \); \( V_s = 13.73 \), and run the neural network approximation of CO dispersion at the level of human respiration (1.5 m) in the entire area of smoke propagation in the case of fixed coefficients (Fig. 8) and in the case of fixed starting coefficients (Fig. 9) using both the results of the experimental measurements and the refined equation.

**Figure 8.** Step 3: Visualized approximation of CO dispersion in the entire area of the smoke propagation, received using the experimental data and the refined equation (fixed coefficients; 1 particle in the cloud; 50 neurons)

**Figure 9.** Step 3: Visualized approximation of CO dispersion in the entire area of the smoke propagation, received using the experimental data and the refined equation (fixed starting coefficients; 1 particle in the cloud; 150 neurons)
Conclusions

Some variants of approaches for constructing a neural network model of CO diffusion from a model source with a burning peat simulating a "smoke geyser" on a peat bog were developed and tested. The model is based on a numerical neural network solution of the atmospheric diffusion equation that realizes the fundamental physical law of matter conservation.

The availability of information on the "fire load" (mass of peat), the burning surface and the concentrations of CO directly above the combustion zone allows to calculate the values of CO, then, – the CO concentration field in the entire area of smoke propagation.

The method is recommended for the development of air quality control and forecasting systems.

The authors are going to devote a separate publication to methods of constructing neural network models for air pollution with other harmful components – the peat fire particles $PM_{2.5} - PM_{10}$.

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