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Modelling the Fields of Pollutant Dispersion in the Atmosphere from Flares

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Abstract

The fields of pollutant dispersion in the air from three operating flare installations at the territory of the Mamontovskoye field in the Nefteyugansk District of the Khanty-Mansi Autonomous Territory were modelled on the basis of climatic data and technological parameters of flare installations. The amounts of pollutants entering the atmosphere from associated petroleum gas combustion were calculated: carbon monoxide (CO) – 83 %, nitrogen dioxide (NO_2) – 0.7 %, soot –10 %, methane – 6 %. The vegetation cover was mapped relying on the Sentinel-2 satellite image with the shooting date of June 14, 2021, displaying dispersion fields for CO, NO_2 and soot. The distances from emission source (flare installation) to isolines with CO and soot concentrations equal to 1 MPC_{st} (5 and 0.15 mg/m^3) are 163 and 505 m, respectively (here MPC_{st} is the maximum permissible concentration for short-term exposure level). Similarly, measured distance to the isoline with NO_2 concentration 0.1 MPC_{st} concentration (0.02 mg/m^3) is 284 m. On average, CO concentration decreases by 1 mg/m^3 at a distance of 86 m and becomes equal to 0.2 mg/m^3 (0.04 MPC_{st}) at a distance of about 572 m. The resulting model for CO dispersion does not contradict MERRA-2 satellite data, according to which the concentration of CO in the vicinity of the flare installation was 0.2 mg/m^3. The gas chromatographic – mass spectrometric analysis of soil samples and plants collected to the north-east from the flare installation at a distance of 216, 486, 710, 1037 and 1380 m has shown that aliphatic hydrocarbons prevail in the composition of soil organic matter. Their content varies from 50 to 80 % of all identified compounds, with the predominance of high-molecular homologues (C_{27}–C_{33}). The maximum total amount of *n*-alkanes (75.3 μg/g) was detected in the soil sample taken at a distance of 710 m from the flare installation. In the organic matter of pine needles and blueberry leaves, C_{27} homologue dominates, and C_{25}, C_{29}, C_{31} characteristic of terrestrial vegetation are present. In addition, polyaromatic compounds were identified in the soil: anthracene/phenanthrene, fluoranthene and pyrene.

Keywords: dispersion fields, concentration isolines, MERRA-2, associated petroleum gas, flare installations, hydrocarbons

INTRODUCTION

The Khanty-Mansi Autonomous Territory – Yugra (KhMAT) is the territory where 43.7 % of Russian oil resources are produced. The amount of associated petroleum gas (APG) produced in the KhMAT in 2021 was 32.8 bln m^3, including 31.4 bln m^3 (95.8 %) extracted and used, while 1.33 bln m^3 (4.1 %) was burnt in flares [1].

Flares at preliminary water discharge units are included in the list of sources of atmospheric pollution over the territory of the KhMAT. It is known [2] that air pollution level is very high in Nizhnevartovsk, the city is included in the Prior-

TABLE 1

Emissions of pollutants in 2019 and 2020 from stationary sources in the cities of the Nefteyugansk District of the KhMAT according to the data reported in [3], t

City	Solid substances		SO_2		CO		NO_2		Hydrocarbons		Volatile organic compounds	
	2019	2020	2019	2020	2019	2020	2019	2020	2019	2020	2019	2020
Nefteyugansk	29	319	105	144	131	310	215	245	2	3	29	114
Pyt-Yakh	47	2208	14	6	2223	20162	985	1256	106	2359	284	1407

ity list of Russian cities with the highest air pollution level. The level of air pollution is high in such cities as Beloyarskiy, Berezovo, Nefteyugansk, Raduzhniy, and Surgut, while it is elevated in Khanty-Mansiysk. An increase in the concentrations of carbon (soot) and formaldehyde has been detected in most of the cities over the Territory during the years 2018–2022, with an especially significant increase observed in Nizhnevartovsk. However, in 2022, a decrease in the concentrations of phenol and nitrogen dioxide (NO_2) is observed in Khanty-Mansiysk and in Nizhnevartovsk. Nefteyugansk has also been included in the list of cities with the high level of atmospheric pollution with such substances as formaldehyde, suspended matter, carbon (soot), phenol, NO_2. Emissions of pollutants into the atmosphere from the industrial enterprises of Nefteyugansk accounted for 50 t of solids, 90 t SO_2, 500 t NO_2, 300 t CO [2]. During 2019 and 2020, the amounts of CO and NO_2 emitted in Pyt-Yakh and Nefteyugansk cities are listed in Table 1 [3]. The amount of NO_2 emitted in Nefteyugansk in 2022 increased by 255 t in comparison with the amount emitted in 2020. The largest amount of pollutants emitted into the atmosphere was detected in 2020 in Pyt-Yakh (see Table 1).

In spite of the emission of pollutants, their concentrations in air are not high [3]. According to the data of the Khanty-Mansiysk Centre for Hydrometeorology and Environmental Monitoring, CO concentrations in Nefteyugansk varied from 0.1 to 0.5 mg/m^3, NO_2 concentrations varied from 0.005 to 0.04 mg/m^3 during the years 2021–2023 (Fig. 1).

The fields of pollutant dispersion in the atmosphere from an enterprise with stationary pollutant sources are modelled by automated calculation of ground-level concentrations of atmospheric pollutants within the boundaries of industrial grounds of enterprises, residential areas, and the areas of sanitary protection [4]. Then the correspondence is determined between the qualitative and quantitative parameters of emissions from enterprises, and the health and safety regulations for air quality in working areas, residential locations, resort and recreation areas.

Satellite-based methods allow evaluation of atmospheric air pollution over separate areas in regions [5] and countries [6–8].

The relevance of the present study is due to the existing emissions of pollutants into the air from stationary sources in oil and gas producing regions, which determines the goal of the work:

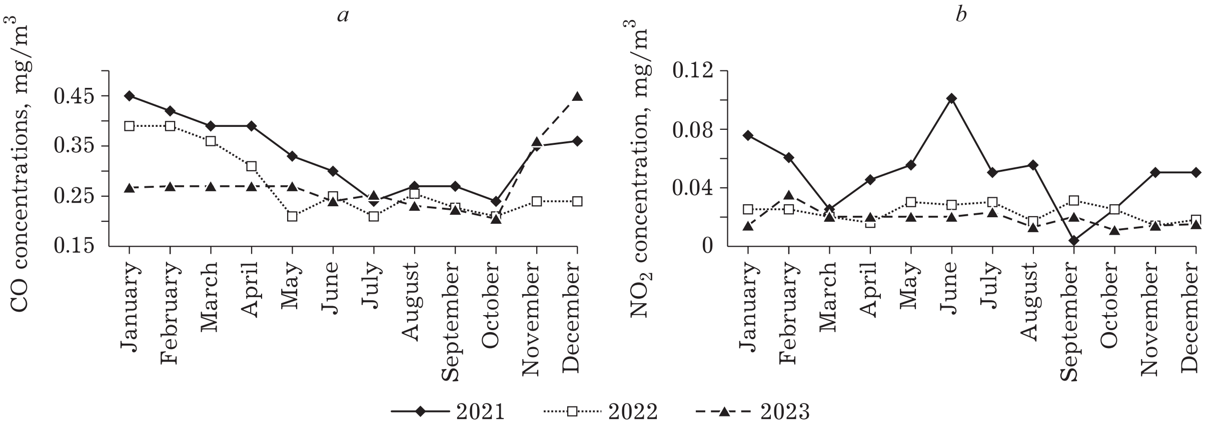

Fig. 1. Concentrations of CO (*a*) and NO_2 (*b*) in Nefteyugansk according to land-based data [3].

modelling of atmospheric dispersion fields for pollutants emitted by flare units (FU) over the territory of the Nefteyugansk District.

The following tasks were solved within the formulated goal:

1) To model dispersion fields for the pollutants: CO, NO_2, methane, soot.

2) To compare the data for CO obtained by modelling with satellite data from MERRA-2.

3) To sample soils and plants at the grounds located in pollutant dispersion fields, and to determine hydrocarbon contents in these samples.

EXPERIMENTAL

Flare units (FU) considered in the work are situated at the territory of the Mamontovskoye oilfield in the Nefteyugansk District of the KhMAT. The area of the Nefteyugansk District is 2 267 951 ha, including 1 245 597 ha of forests. The forests relate to the West Siberian middle taiga plain forest region of the taiga zone with predominance of forest with grass layer and deciduous forest [9]. The studies show [5] that northern forests are prone to thermal and aerosol pollution from operating FU in which APG is burnt at the oil and gas producing objects. The regions of oil-polluted land in the Nefteyugansk District of the KhMAT exhibiting a very high pollution degree with petroleum product concentration 70–145 times higher than the tentative permissible level were revealed previously in [10]. The flares are installed within the preliminary water discharge units at the Mamontovskoye oilfield under development by the RN-Yuganskneftegaz company (PJSC Rosneft). The Mamontovskoye oilfield is situated in the central part of the West Siberian Plain, in the Salym-Ob plain terrace bog-taiga landscape province. Preliminary water discharge units operate by discharging water to its residual content in oil about 1–10 %. Gas separation is performed, and a part of the gas is directed to compressor station and then enters the gas processing plant. Residual gas is directed to low-pressure flare for combustion [11].

Modelling of CO dispersion fields was carried out in the unified software package for calculating atmospheric pollution UPRZA OND-86 of December 24, 2018, which is available on the Internet and has been developed by PC ECO center [12] on the basis of regulatory document [13]. This regulatory document was transformed in 2017 into the methods to calculate dispersion of the emissions of hazardous (pollutant) substances in atmospheric air [14].

Parameters for modelling dispersion fields in UPRZA OND-86 software are: mouth diameter and height of a point source; temperature, outlet velocity, and the volume flow rate of gas-air mixture; maximum short-time and overall emission of a pollutant. The maximal volumes of APG to be burnt were determined according to [11].

To carry out modelling using the UPRZA OND-86 software, additional calculations were carried out according to the procedure described in [15].

The volume flow rate of APG burnt in the FU within one second (W_v, m^3/s) is calculated using equation:

$$W_v = W/(t_{day} t_s) \qquad (1)$$

where t_{day} is time of FU operation, days; t_s is the number of seconds in 24 h ($24 \cdot 3600$); W is volume flow rate of gas burnt at the FU per year, m^3/year.

The volume flow rate of combustion products leaving the FU (W_{pr}, m^3/s) is calculated using equation:

$$W_{pr} = W_v V_{cp} \cdot ((273 + T_g)/273) \qquad (2)$$

where W_v is the volume flow rate of APG burnt at the FU during 1 second, calculated using equation (1), m/s; T_g is combustion temperature, °C; V_{cp} is the amount of combustion products formed in stoichiometric combustion of 1 m^3 of APG in humid air, as calculated in [16], m^3/m^3.

The average rate at which the products of APG combustion enter the atmosphere (W_{cp}, m/s) is calculated as:

$$W_{cp} = 1.274\ W_{pr}/D_f^2 \qquad (3)$$

where D_f is the flare diameter calculated in [16], m.

Calculation of the maximal emissions of hazardous substances (W_{gi}, g/s) is performed using the equation:

$$W_{gi} = 0.278 q_i\ W_g \qquad (4)$$

where q_i is a specific emission of an i^{th} hazardous substance per unit mass of gas for combustion, kg/kg; W_g is the mass flow rate of gas discharged at the flare unit, kg/h, determined using the equation:

$$W_g = 3600 \rho_g W_v \qquad (5)$$

where ρ_g is gas density, kg/m^3.

Calculation of overall emissions of hazardous substances per year ($W_{gi}(t)$, t/y) is carried out using the equation:

$$W_{gi}(t) = 0.001 q_i W_g t \qquad (6)$$

where t is the time of FU operation per year, h.

Calculated maximum short-time and overall emissions from three FU at the Mamontovskoye

TABLE 2

Maximal short-term and overall emissions from the studied flare units (FU)

Component	CO	NO_2	Soot	Benz(a)pyrene	Methane
		FU No. 1			
Maximal emissions, g/s	13.815	0.1105	1.658	$4.42 \cdot 10^{-9}$	0.995
Overall emissions, t/y	435.32	3.48	52.239	$1.393 \cdot 10^{-7}$	31.34
		FU No. 2			
Maximal emissions, g/s	57.17	0.457	6.87	$1.83 \cdot 10^{-8}$	4.116
Overall emissions, t/y	93.77	0.75	11.25	$3 \cdot 10^{-8}$	6.75
		FU No. 3			
Maximal emissions, g/s	10	0.08	1.2	$3.2 \cdot 10^{-9}$	0.72
Overall emissions, t/y	315.22	2.52	37.82	$1 \cdot 10^{-7}$	22.7

oilfield in the KhMAT are shown in Table 1. The amounts of pollutants that enter the atmosphere from APG combustion were calculated using the obtained data: CO – 83 %, soot – 10 %, NO_2 – 0.7 %, methane – 6 %.

One of the satellite-based methods to study CO concentration in the atmosphere is MERRA-2. This is atmospheric re-analysis (repeated analysis) with spatial resolution 0.5° × 0.625°, performed by the Global Modelling and Assimilation Office (GMAO) of the National Aeronautics and Space Administration of the USA (NASA) [17].

Soil was sampled in 2021 in the zone affected by FU No. 3 in order to determine the concentrations of pollutants. Samples were collected, taking into account the wind rose over the territory under investigation. Five soil samples (Fig. 2, A, B, C, D, and E) were taken from the surface of grounds located at different distances from FU (A – 216, B – 486, C – 710, D – 1 037, E – 1 380 m). Pine needles and the leaves of blueberry were also sampled from ground B. The organic matter was isolated from dried soil (2–20 g) by extraction with a 7 % solution of methanol in chloroform at 65 °C for 2 h. The hydrocarbon fraction was separated from the organic matter using hexane. Detailed analysis of the hydrocarbon fraction was carried out using a DFS gas chromatograph – mass spectrometer (Thermo Scientific, Germany).

RESULTS AND DISCUSSION

The emissions include CO, NO_2, soot, benz(a) pyrene, methane. The compound prevailing in emissions is CO: 435.32 t/y from FU No. 1, 93.77 t/h from FU No. 2, 315.22 t/y from FU No. 3.

The isoline from FU No. 1 and FU No. 2 with CO concentration is equal to 5 mg/m^3 (or, expressed in fractions of the maximal short-term permissible concentration (MPC_{st}), – 1 MPC_{st}) and goes at a distance of 290 m. The isoline with NO_2 concentration equal to 0.02 mg/m^3 (0.1 MPC_{st}) is at a distance of 625 m from the FU. Modelling of soot concentration fields revealed excess over MPC_{st}. At a distance of 722 m, 3 MPC_{st} was detected (0.45 mg/m^3), however, at the boundary of the sanitary protection zone (1 km from the FU) soot concentration does not exceed 1 MPC_{st}.

Isolines of CO concentration from FU No. 3 imposed on the vegetation map that has been generated on the basis of satellite image (SI) from Sentinel-2 taken on 14.06.2021 are shown in Fig. 2. The distances from FU No. 3 to isolines with CO concentration 1 MPC_{st} (5 mg/m^3) and 0.2 MPC_{st} (1 mg/m^3) are 163 and 508 m (see Fig. 2). The distances from FU No. 3 to the isoline with NO_2 concentration equal to 0.1 MPC_{st} (0.02 mg/m^3) is 284 m, to the isoline with soot concentration equal to 1 MPC_{st} (0.15 mg/m^3) – 505 m (see Fig. 2).

Dispersion fields for methane and benz(a)pyrene were not calculated because of their very low concentrations.

With an increase in the distance from FU, the concentrations of pollutants in the atmosphere decrease. No excess over MPC_{st} of pollutants was detected within the boundaries of summer residence places situated to the south from FU-3 (see Fig. 2).

Results obtained by CO dispersion field modelling do not contradict with satellite observations. The map of CO concentrations corresponding to sampling day 28.09.2021 (Fig. 3) was generated on the basis of MERRA-2 SI. The objects burnt in 2023, according to the data of the web portal [18] are mapped as a layer of points. The accumulations of thermal points were identified according to the data of the web portal [19], with subsequent determination of FU coordinates. One can see (see Fig. 3) that the highest CO concentrations within the range of 126–129 ppbv (0.148–

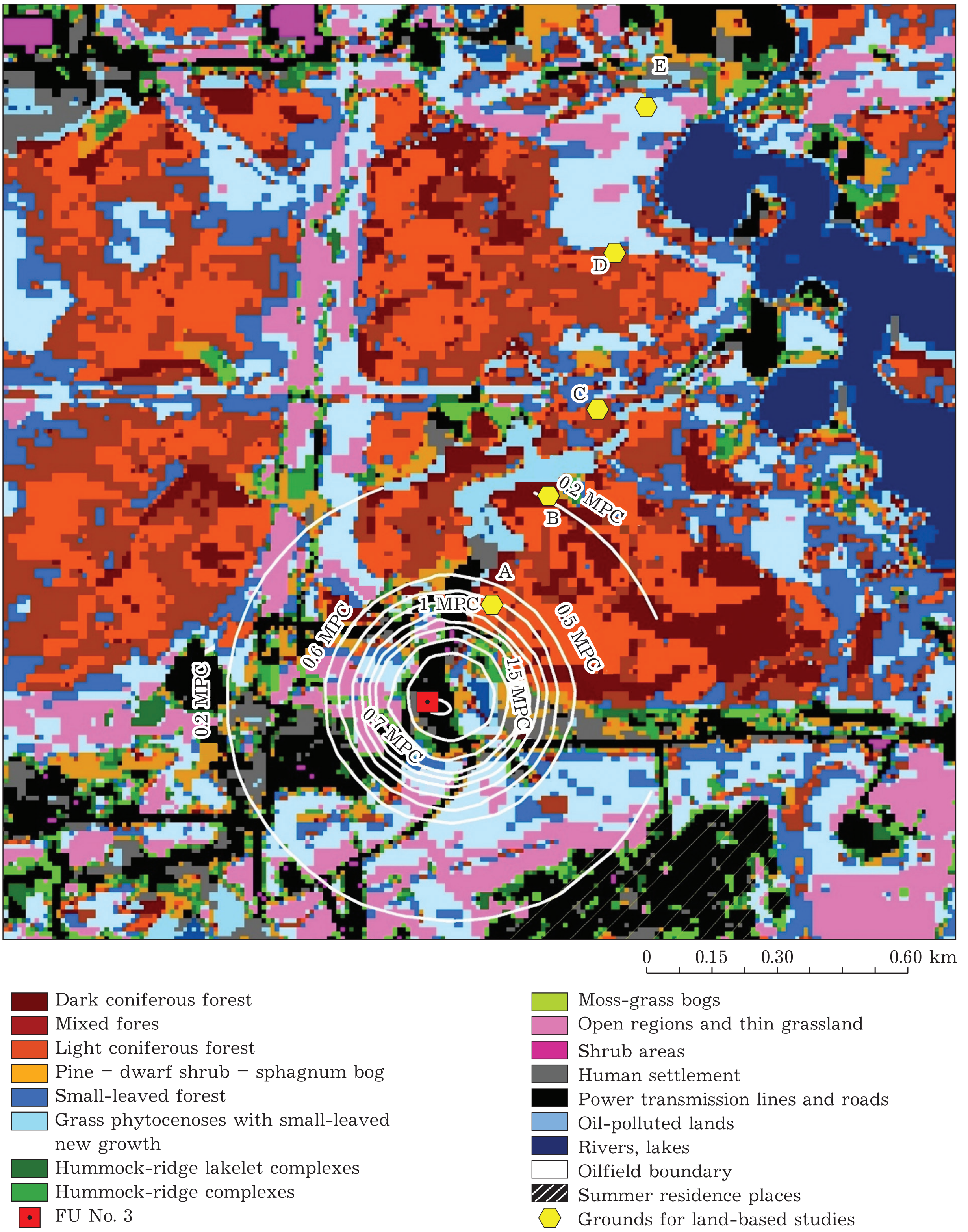

Fig. 2. CO dispersion fields in atmospheric air around flare unit No. 3 (FU No. 3) at the Mamontovskoye oilfield. Letters (A, B, C, D, E) mark the grounds from which soil and plants were sampled. MPC – maximal permissible concentration, PTL – power transmission lines.

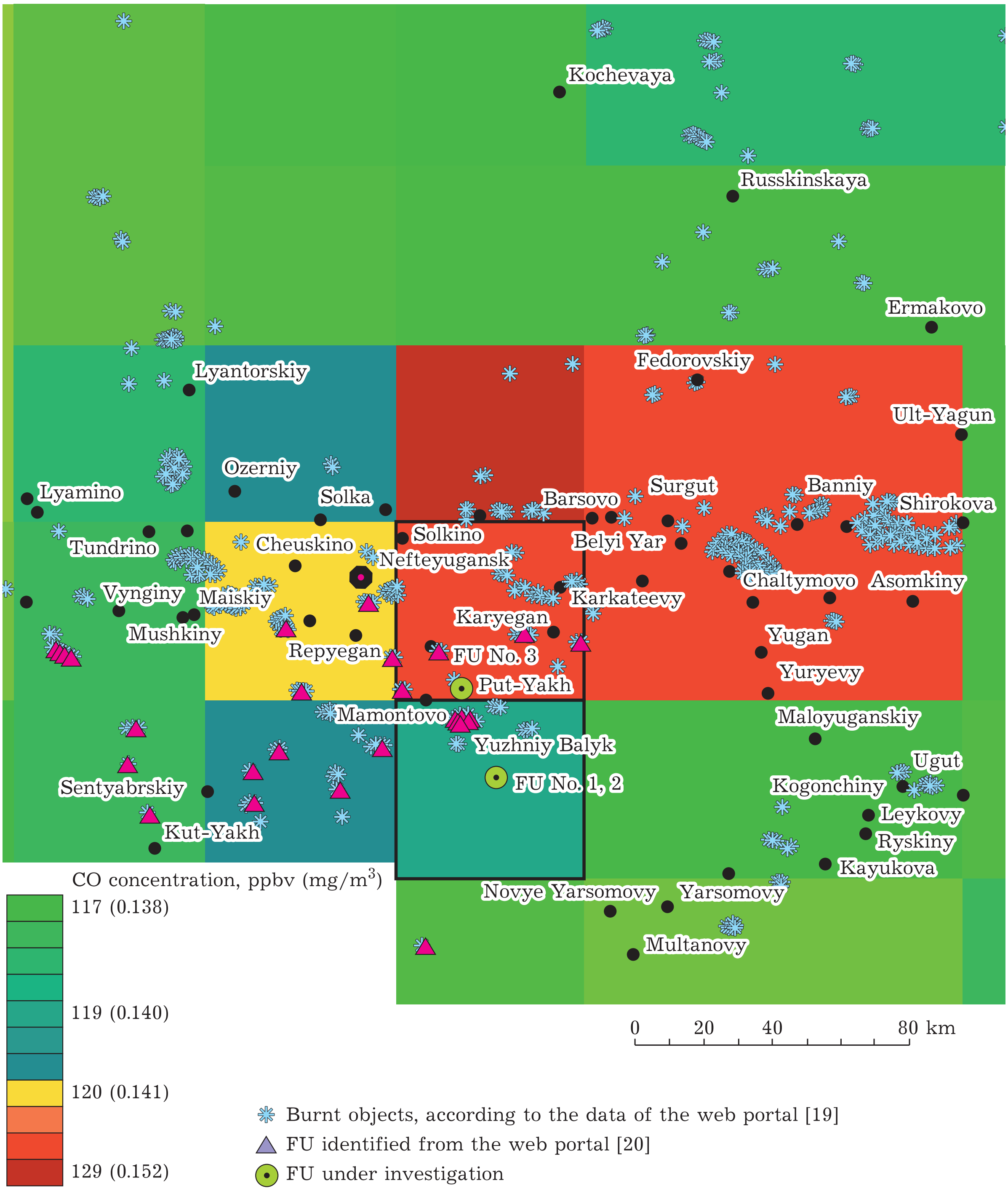

Fig. 3. Map of CO concentrations compiled from MERRA-2 satellite image, on 28.09.2021. FU – flare unit.

0.151 mg/m^3) are observed in the squares marked with red colour, where the cities Nefteyugansk, Pyt-Yakh, Surgut, Beliy Yar. The concentrations of CO are not high on all grounds, they are equal to 0.03 MPC$_{st}$ (0.2 mg/m^3) on average.

Organic compounds that were identified in soils and plants with the help of gas chromatographic – mass spectrometric analysis over molecular masses (m/z) include n-alkanes and isoalkanes (m/z 57), hopanes, hopenes and oleanenes (m/z 191), steranes (m/z 217, 218), anthracene (m/z 178), fluoranthene and pyrene (m/z 202), chlorophenothanes (m/z 235).

The molecular mass distribution of n-alkanes in soil and in plants over the territory under investigation is shown in Fig. 4.

Gas chromatographic – mass spectrometric analysis showed that the traces of hydrocarbons

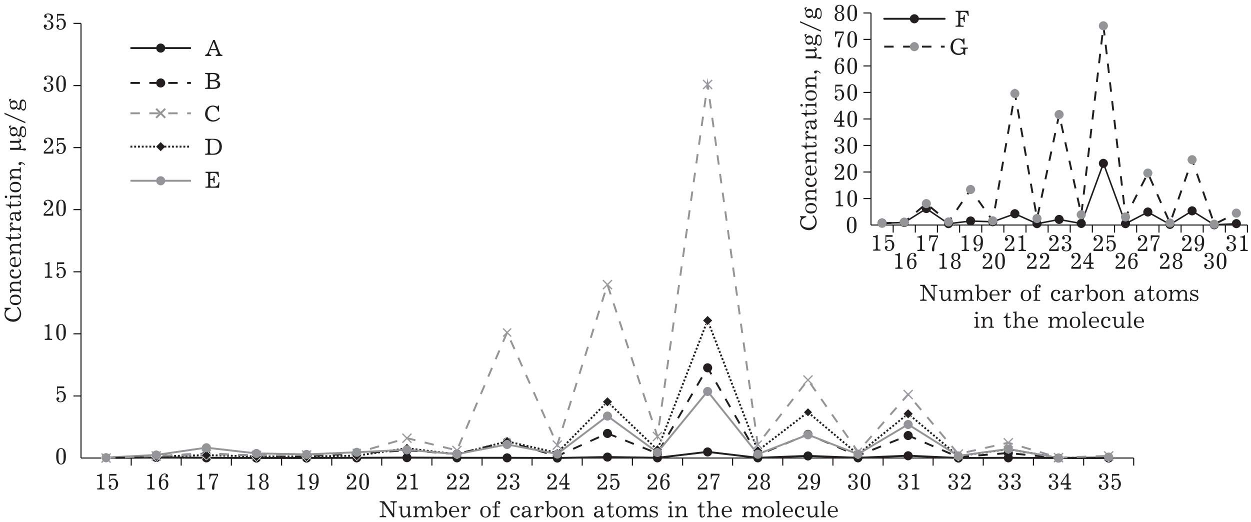

Fig. 4. Molecular mass distribution of *n*-alkanes in soil. Location of grounds (A–E) for soil sampling is shown in Fig. 2. The insert shows the concentrations of *n*-alkanes in pine needles (F) and in the leaves of blueberry (G) at a distance of 486 m from the flare unit.

were detected in the organic matter of plants sampled from ground B. Aliphatic hydrocarbons prevail in the composition of soil organic matter: their content varies from 50 to 80 % of all identified compounds, with domination of high-molecular homologues (C_{27}–C_{33}). The maximal total content of *n*-alkanes was detected in the sample taken from ground B (75.3 µg/g) at a distance of 710 m from FU, and minimal one – in the sample taken from ground A (1.21 µg/g). The homologue dominating in soils sampled from the flare-affected zone at a distance up to 1500 m is C_{27}, in addition, substantial fractions are those of homologues C_{25}, C_{29}, C_{31}, characteristic of land vegetation [20].

Besides, polyaromatic hydrocarbons (PAH) were identified in soil: anthracene/phenanthrene, fluoranthene and pyrene, which are likely to be formed in gas combustion in FU. Their distribution, shown in Fig. 5, points to an increase in the concentration with an increase in the distance from the pollution source. The maximal PAH content is observed in the sample taken at a distance of 1380 m from the flare, which may be due to their combustion, subsequent dispersion in the atmosphere, and deposition on soil. Besides, the samples were determined to contain monounsaturated compounds – hopenes and oleanenes, which are characteristic of natural substances [21].

Chlorophenothanes, substances incorporated in insecticides used against forest pests, were detected in all soil samples except background ones. The content of these compounds is higher than MPC_{st} (the MPC_{st} of chlorophenothanes in soil is 0.1 µg/g [22]) by a factor of 11–184, except sample A. This compound is likely to get into soil from the air.

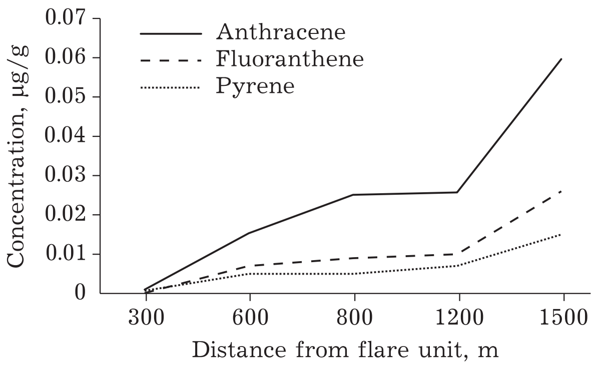

Fig. 5. Distribution of polyaromatic hydrocarbons in the zone affected by the flare unit.

In general, modelled concentrations of CO, NO_2, soot do not exceed 1 MPC at the boundary of the sanitary protective zone (1000 m) around one flare. According to the MERRA-2 satellite data, CO concentration is not high in the region of Nefteyugansk and Pyt-Yakh, it is equal to 0.03 MPC_{st} (0.15 mg/m^3) on average.

With an increase in the distance from FU, the amount of hazardous substances decreases due to dispersion from high-altitude sources. Combustion products from FU that are characteristic of the combustion of organic fuel have been determined in soil. Gradual increase in PAH content with an increase in the distance from the flare is observed, which does not exclude possible migration of pollutants from Pyt-Yakh and their deposition in the upper layers of peaty soil. Chlorophenothane in the concentration several ten times higher than the MPC_{st} was detected in soils.

CONCLUSION

Thus, the approach based on modelling the fields of pollutant dispersion in atmospheric air from FU is proposed in the work, involving a complex of technological and climatic parameters, regulatory documents, software, remote and on-land data. A computer map of vegetation cover has been composed on the basis of Sentinel-2 SI taken on 14.06.2021 and depicting these fields. The distances from FU No. 3 to isolines with the concentrations equal to 1 MPC_{st} (for CO), 0.1 MPC_{st} (for NO_2) and 1 MPC_{st} (for soot) are 163, 284 and 505 m, respectively. On average, CO concentration decreases by 1 mg/m^3 at a distance of 86 m and is equal to 0.2 mg/m^3 at a distance of about 572 m. The compiled model of CO dispersion fields does not contradict the MERRA-2 satellite data. On 28.09.2021, CO concentration in the vicinity of FU was 0.2 mg/m^3. Analysis by gas chromatography – mass spectrometry shows that aliphatic hydrocarbons prevail in the composition of organic matter of soil. Their concentrations vary from 50 to 80 % of all identified compounds, with the domination of high-molecular homologues (C_{27}–C_{33}). The maximal overall concentration of n-alkanes (75.3 μg/g) was detected in the sample taken at a distance of 710 m from the FU. The homologue dominating in pine needles and the leaves of blueberry is C_{27}, and C_{25}, C_{29}, C_{31} alkanes characteristic of and vegetation are present. In addition, PAH were identified in soil, in particular anthracene/phenanthrene, fluoranthene and pyrene.

The developed approach allows carrying out monitoring-based studies of the state of environment over remote northern oil and gas producing territories.

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