FASO RUSSIA FEDERAL RESEARCH CENTRE
«KOLA SCIENCE CENTRE OF THE RUSSIAN ACADEMY OF SCIENCE»
Institute of North Industrial Ecology Problems

Modelling approaches

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INEP (Institute of Industrial Ecology Problems in the North, Kola Science Center, RAS) & UHEL-INAR (University of Helsinki, Institute for Atmospheric and Earth System Research)

Lab. for Interdisciplinary Environmental and Economic Studies

The main directions of scientific activities of the laboratory

- development of mathematical models of atmospheric dynamics and cluster analysis of possible trajectories of atmospheric transport of pollutants in the Arctic;
- assessment of the environmental consequences of airborne industrial pollution using space monitoring methods and mathematical modeling;
- study of physical and chemical processes occurring during storage of mining industrial waste;
- research and computer modeling of oil degradation processes in the modern environment and further transformation of degradation products in natural waters;
- study of the formation of the chemical composition of sea and fresh waters in the "water - rock" systems depending on the composition of the rocks;
- determination of the forms of migration of elements in waters, atmospheric precipitation using physical and chemical modeling;
- physical and chemical modeling of natural and technological processes aimed at solving scientific and applied problems in the field of mineral formation, chemistry and chemical technology, geoecology.

Lab. for Interdisciplinary Environmental and Economic Studies

The main directions of scientific activities of the laboratory

Last three years we expanded our research to study of:

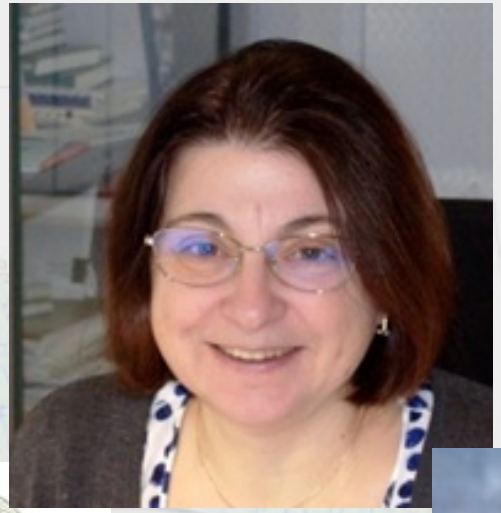
- creation of medico-geochemical maps and identification of cause-and-effect relationships between population health and geochemical landscapes (chemical composition of surface and underground waters);

- development of economic and political mechanisms for greening economic activity in the Arctic zone of the Russian Federation;

- methodological approaches to calculating economic damage to the health of the Arctic population from industrial pollution

Leading Scientists of Lab.

Vladimir Masloboev
Dr. of Sc.
(Engineering)



Elena Klyuchnikova
PhD (Economics)

Svetlana Mazukhina
Dr.of Sc.
(Geology &
Mineralogy)

Pavel Amosov
PhD (Engineering)

Fidel Pankratov
PhD (Geography)

CFD-MODELING OF DUST TRANSFER

Governing equations

The model of incompressible liquid and the standard (*k*-*ε*)-model of turbulence

$$\rho\frac{\partial \mathbf{U}}{\partial t} - \nabla \cdot \left[\left(\eta + \rho C_\mu \frac{k^2}{\varepsilon}\right) \cdot (\nabla \mathbf{U} + (\nabla \mathbf{U})^T)\right] + \rho \mathbf{U} \cdot \nabla \mathbf{U} + \nabla P = \mathbf{F}$$

$$\nabla \cdot \mathbf{U} = 0$$

$$\rho\frac{\partial k}{\partial t} - \nabla \cdot \left[\left(\eta + \rho\frac{C_\mu k^2}{\sigma_k \varepsilon}\right)\nabla k\right] + \rho \mathbf{U} \cdot \nabla k =$$

$$= \rho C_\mu \frac{k^2}{2\varepsilon} (\nabla \mathbf{U} + (\nabla \mathbf{U})^T)^2 - \rho\varepsilon$$

$$\rho\frac{\partial \varepsilon}{\partial t} - \nabla \cdot \left[\left(\eta + \rho\frac{C_\mu k^2}{\sigma_\varepsilon \varepsilon}\right)\nabla \varepsilon\right] + \rho \mathbf{U} \cdot \nabla \varepsilon =$$

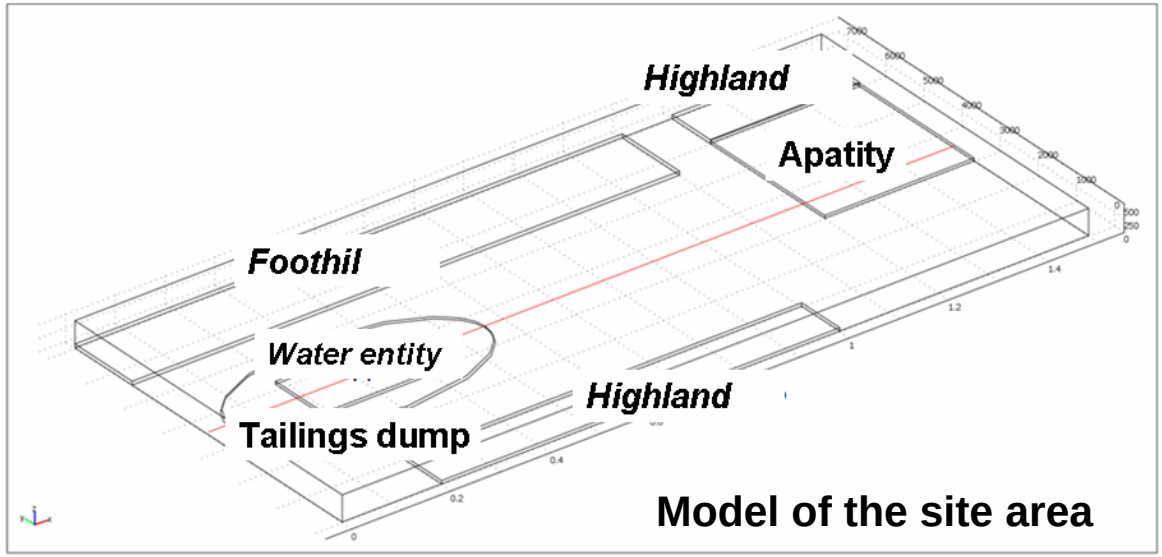
$$= \rho C_{\varepsilon 1} \frac{k}{2} (\nabla \mathbf{U} + (\nabla \mathbf{U})^T)^2 - \rho C_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

Advection-diffusion transfer

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i + c_i \mathbf{u}) = R_i$$

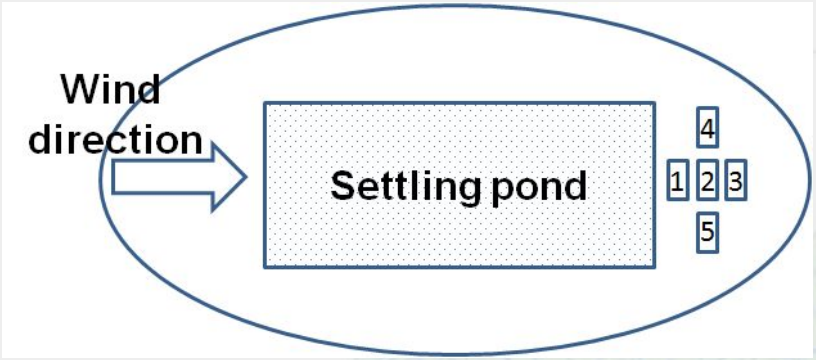
COMSOL software

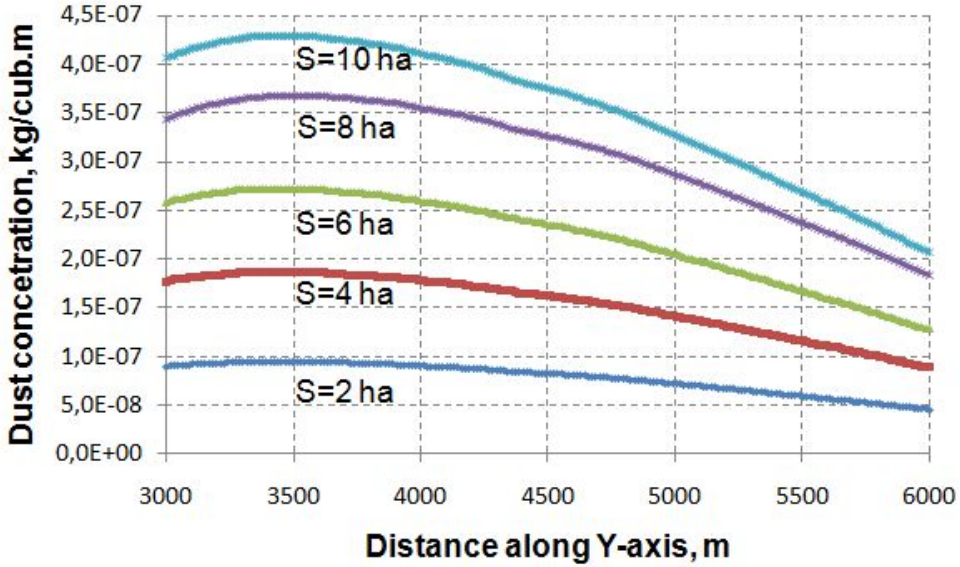
Grid for digital imaging of the site area



Model of the site area

ESTIMATION OF AIR POLLUTION LEVELS BY NUMERICAL MODELING DEPENDING ON WIND FLOW SPEED AND DUSTING SOURCE AREA



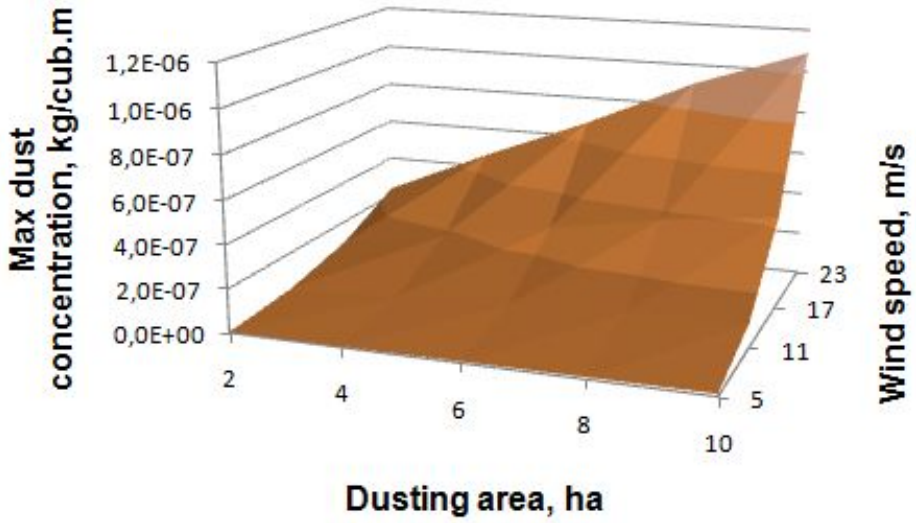


Wind flow speed V — 5, 11, 17 and 23 m/s

Dusting source area S — 2 ha (plot 1), 4 ha (plots 1-2), 6 ha (plots 1-3), 8 ha (plots 1-4) and 10 ha (plots 1-5)

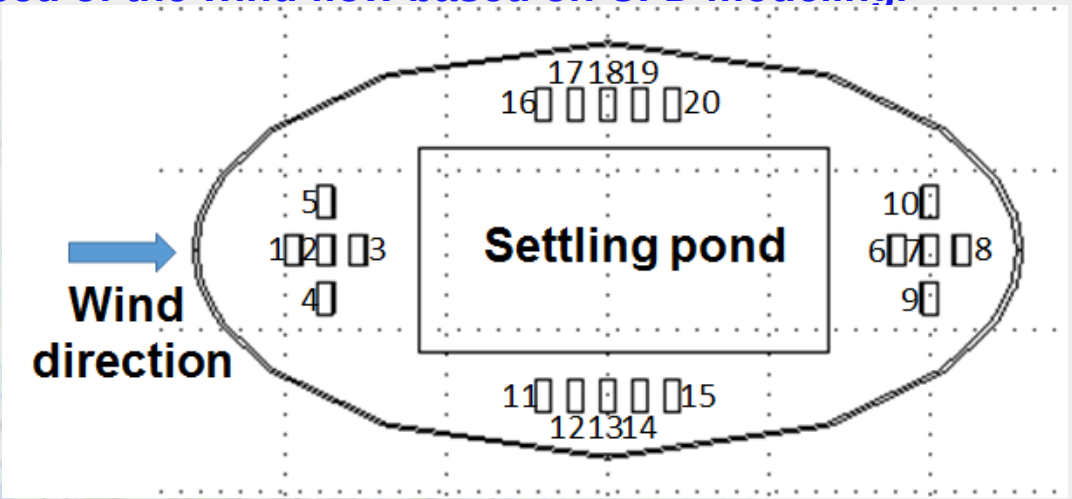
The maximum concentration of dust in the atmosphere, kg/m^3

$$C_m = 10^{-12} \cdot (9.510 \cdot S + 1.932) \cdot V^{2.975}.$$



Tasks to next 2 years

1. **Evaluation of the levels of pollution of the atmosphere with fine dust in the conditions of dusting of the tailing dump with variations in the location of the sites and the area of the dusty surface, as well as the speed of the wind flow based on CFD modeling.**

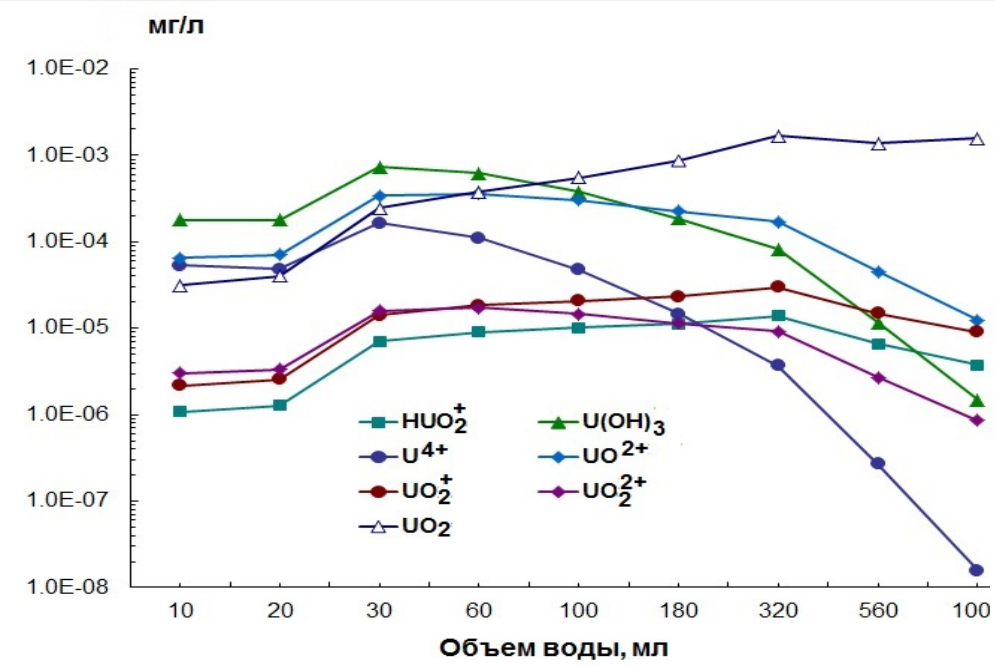


2. **Investigation of the possibility of using the background stratification approach as applied to the problem of modeling dusting processes based on the COMSOL computer code (in a two-dimensional setting).**

3. **Investigation of the influence of meteorological conditions (wind speed, background stratification parameter, etc.) on the intensity of dusting and pollution of the atmospheric boundary layer at technogenic objects of the mining complex of the Arctic region of Russia on the basis of three-dimensional numerical modeling.**
Numerical experiments are supposed to be performed on the basis of the METEO / TRANS model package (IPPES KSC RAS). To simulate the transfer of multi-particulate dust, the TRANS block will be modified.

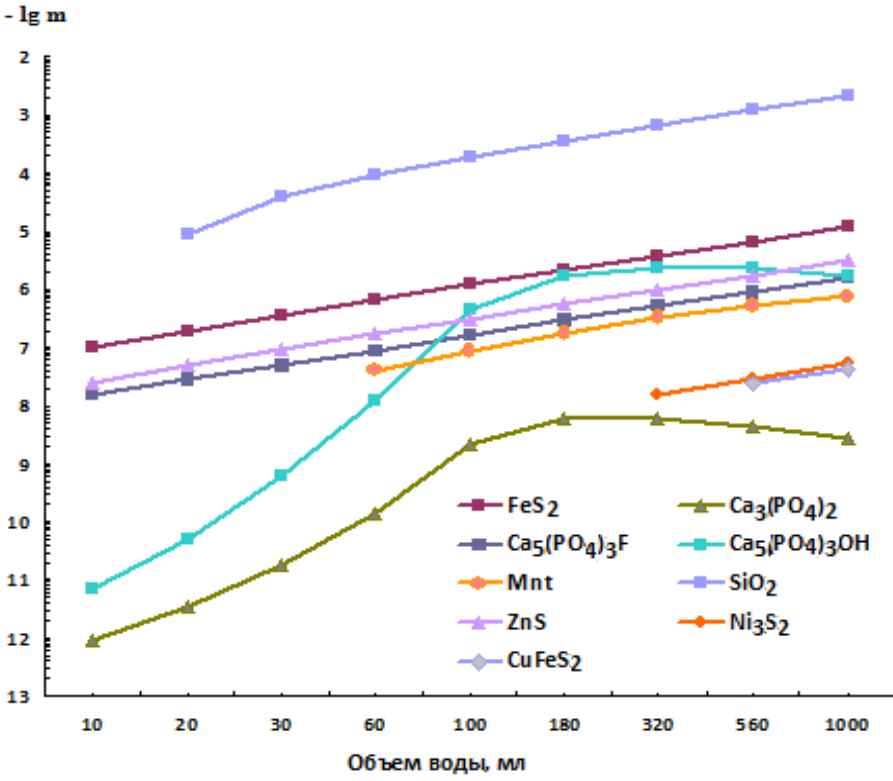
Thermodynamic approach

The method of physicochemical modeling (PC Selector) is based on the minimization of thermodynamic potentials. This method makes it possible to study the "solution-rock" systems in the environment and physiological environments of the human body, where "solution" is natural waters, drinking water, gastric juice, a mixture of drinking water and gastric juice, and "rock" is the rocks of the studied areas or the composition of newly formed phases in equilibrium with a solution within a single multisystem. Such an approach, without simplifying the multisystem, will make it possible to determine the chemical forms of migration of elements in the system "natural waters - gastric juice" under conditions of low and high acidity, conditions for the precipitation of mineral phases that can be transported from the stomach to other organs and tissues; to reveal the forms of migration of rare earth elements, since the ions of the latter are able to replace not only alkaline earth ions, but also transition metal ions, while replacing similar ones with alkaline earth ions is impossible. Thus, the applied approach opens up new perspectives in environmental and medico-environmental research.

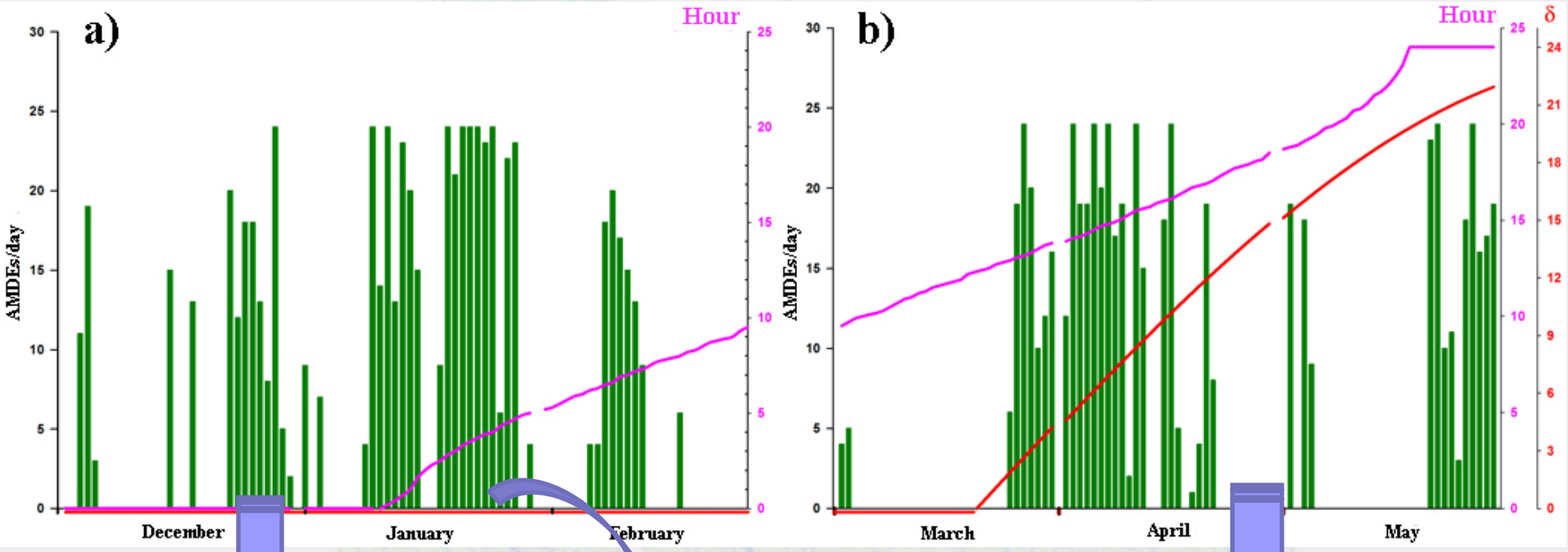


Formation of solid phases (m - mol) with a change in the volume of spring water in system, the volume of gastric juice is 100 ml, T = + 38oC, P = 1 bar, initial values pH = 6.24, Eh = - 0.218 V.

Forms of uranium migration during the interaction of 100 ml of gastric juice and waters of spring No. 1 when the volume of water in the system changes from 10 to 1000 ml



Number of decreased values of mercury concentration in the atmosphere during the day December-January 2010-2011 (a) and March-May 2011 (b)



AMDEs = 32

T_{max} = 28 hours

AMDEs – 18

T_{max} = 46 hours

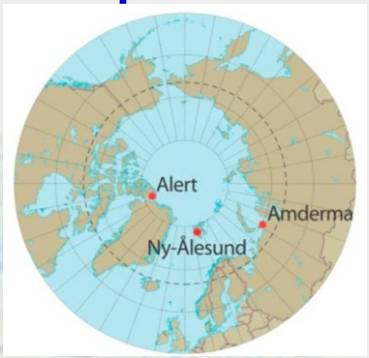
AMDEs = 21

T_{max} = 66 hours

Pilot Study:
Assessment of the impact of potential source regions on environmental pollution in the Arctic regions due to mercury atmospheric transport of mercury

- **Mercury (Hg) long-term measurements:**

  Amderma polar station (69°45'32'' N latitude,
  61°40‘44'' E longitude,
  53.5 meters asl)



International polar station at the Northern Hemisphere

- **Research Tools:**

  (1) ***trajectory modeling approach*** (NOAA HYSPLIT) to calculate backward trajectories and cluster analysis to assess dominating directions of mercury atmospheric transport on annual and seasonal scales ;

  (2) ***online integrated approach*** (Enviro-HIRLAM) for meteorology–atmospheric composition modeling to simulate atmospheric transport, dispersion and deposition of pollutants for:
  (a) periods of intense Icelandic volcanic activity (including mercury emissions)
  (b) short-term episodes of black carbon elevated emissions

  in order to assess potential impact on environment and population of Arctic regions.

- **Developments:**
  - **Hg-module**: refine chemical kinetics and photochemical data reaction Hg taking into account molecular weight, diffusivity, partitioning coefficients among octanol, water, and air of Hg related compounds, including $HgCl_2$, $HgBr_2$, HgO, $Hg(NO_3)_2$, $HgSO_4$, etc;
  - **Preprocessing** module for local meteorology;
  - **Test** as a stand-alone module and **implement** into Enviro-HIRLAM model.


Thank you for attention!