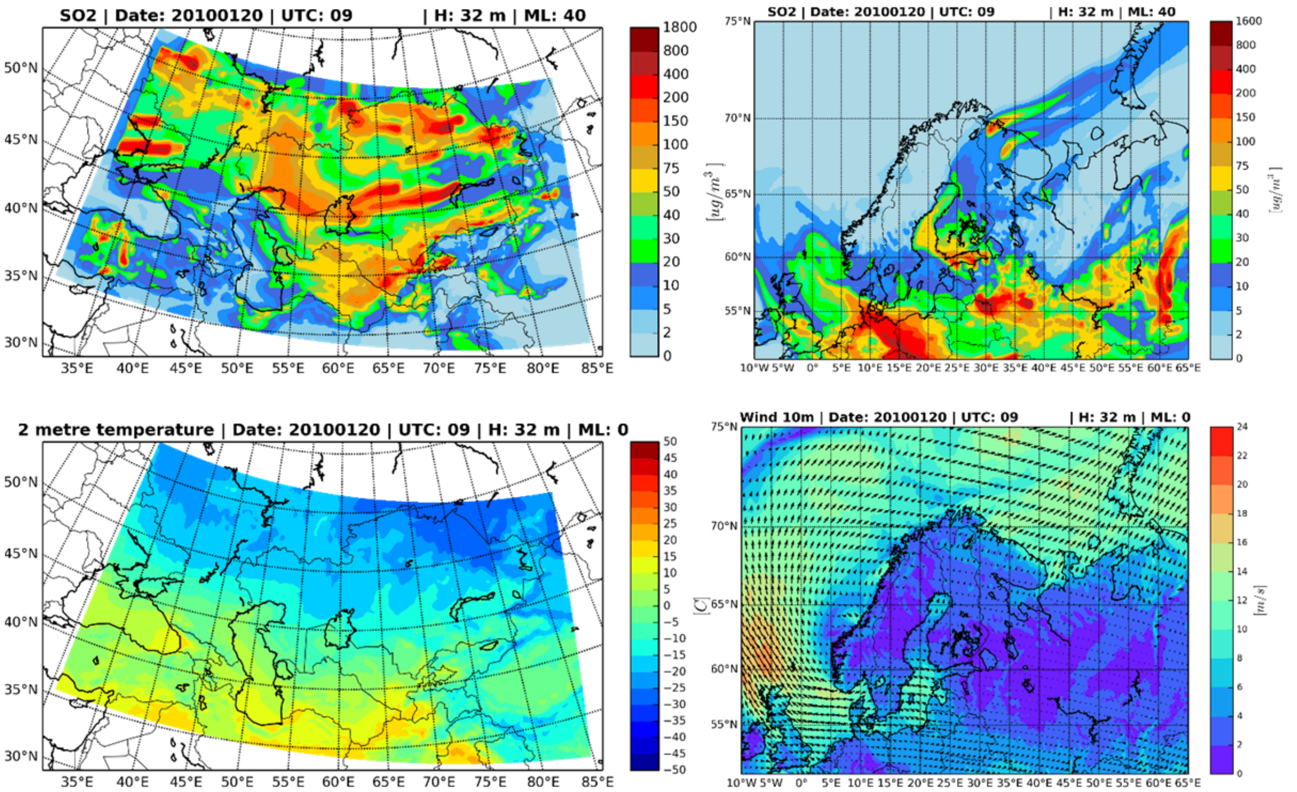
DMI
Danish Ministry of Climate, Energy and Building

Scientific Report 15-06

On-line Meteorology-Chemistry/ Aerosols Modelling and Integration for Risk Assessment: Case Studies

Kairat Bostanbekov [1,3]. Alexander Mahura [2]. Roman Nuterman [4,5], Daniyar Nurseitov [1], Edige Zakarin [6], Alexander Baklanov [2,7]

[1] *Kazakh National Research Technical University, Almaty, Kazakhstan*
[2] *Research Department, Danish Meteorological Institute, DMI, Lyngbyvej 100, DK-2100 Copenhagen Ø, Denmark*
[3] *International University of Information Technologies, Almaty, Kazakhstan*
[4] *University of Copenhagen, Niels Bohr Institute, Copenhagen, Denmark*
[5] *Tomsk State University, Tomsk, Russia*
[6] *EcoRisk, Almaty, Kazakhstan*
[7] *World Meteorological Organization, Geneva, Switzerland*



Copenhagen 2015

Dmi
Danish Ministry of Climate, Energy and Building

Colophon

Serial title:
Scientific Report **15-06**

Title:
On-line Meteorology-Chemistry/ Aerosols Modelling and Integration for Risk Assessment: Case Studies

Subtitle:

Author(s):
Kairat Bostanbekov, Alexander Mahura, Roman Nuterman, Daniyar Nurseitov, Edige Zakarin, Alexander Baklanov

Other contributors:

Responsible institutions:
Kazakh National Research Technical University, KazNRTU
Research Department, Danish Meteorological Institute, DMI

Language:
English

Keywords:
Risk assessment, accidental and continuous emissions, sulphur dioxide, Enviro-HIRLAM

Url:
www.dmi.dk/dmi/sr15-06.pdf

Digital ISBN:
978-87-7478-664-1

ISSN:
1399-1949 (on-line)

Version:

Website:
www.dmi.dk

Content:

Abstract

In this study, the Enviro-HIRLAM (Environment - High Resolution Limited Area Model) was adapted and employed for assessment of scenarios with accidental and continuous releases of emissions of sulphur dioxide (SO_2) for selected case studies during January of 2010. The following scenarios were considered: (i) control reference run; (ii) accidental release (due to short-term 1 day fire at oil storage facility) occurred at city of Atyrau (Kazakhstan) near the northern part of the Caspian Sea; and (iii) doubling of original continuous emissions from three locations of metallurgical enterprises on the Kola Peninsula (Russia). The implemented aerosol microphysics module M7 uses 5 types – sulphates, sea salt, dust, black and organic carbon; as well as distributed in 7 size modes. Removal processes of aerosols include gravitational settling and wet deposition. As the Enviro-HIRLAM model is the on-line integrated model, both meteorological and chemical processes are simultaneously modelled at each time step.

The modelled spatio-temporal variations for meteorological and chemical patterns are analyzed for both European and Kazakhstan regions domains. The results of evaluation of sulphur dioxide concentration and deposition on main populated cities, selected regions, countries are presented employing GIS tools. As outcome, the results of Enviro-HIRLAM modelling for accidental release near the Caspian Sea are integrated into the RANDOM (Risk Assessment of Nature Detriment due to Oil spill Migration) system.

1. Introduction

On regional level, and especially in areas with potential diverse sources of industrial pollutants, the risk assessment of impact on environment and population is critically important. During normal operations, the risk is minimal. However, during accidental situations, the risk is increased due to releases of harmful pollutants into different environments such as water, soil, and atmosphere where it is following processes of continuous transformation and transport.

Pollution of the atmosphere by industrial emissions leads to a deterioration of the ecological situation in both the surrounding areas and over the long distances from the location of the emission source. The steel-production plants as well as oil and gas industry can bring a significant effect to air pollution, mainly through burning of associated gases in flare devices. Gas combustion products are quite toxic mixture. For the high-sulfur oil a predominant role in the pollution plays the sulfur dioxide (SO_2). Furthermore, this gas is a major air pollutant among gases in emissions coming from thermal power stations that work through burning coal.

One of territories with sources of emission of large amounts of pollutants, such as SO_2, is the Atyrau region of the Republic of Kazakhstan, where the oil and gas and other industrial enterprises of the country are concentrated. The main purpose of this paper is to analyze the transboundary atmospheric transport and deposition of pollutants from the Atyrau region, as well as to make an assessment of the impact on the territory of neighboring countries. This study investigates the spread of sulfur dioxide in accidents in the oil storage tanks located in the Atyrau region. This area, which is located on the shores of the Caspian Sea, is the industrialized oil-producing region of Kazakhstan.

Many international research projects implemented models and methods that describe the individual parts of the risk assessment, for example, probabilistic safety assessment, long-distance transport and modeling of pollution, radioecological sensitivity, dose assessment, etc. Simulation of spatio-temporal chemical fields and weather forecast has become increasingly popular in the scientific community. There are two modeling approaches for predicting chemical weather: online and offline approaches. The calculation of the spread of sulfur dioxide in the selected regions of the Northern Hemisphere was carried out with the use of the Enviro-HIRLAM online modelling system. As a result of these calculations a large data set was obtained and which was treated with a help of a specially developed procedure. The main purpose of this paper is to analyze the spread of pollutants, based on the short-term modeling to assess the temporal and spatial variability of atmospheric transport in the selected area, and using the modelling results to integrate into GIS environment for risk and vulnerability mapping.

The results of this study can be used to analyze potential impact from atmospheric pollution. The calculation results are presented and summarized in the form of maps and diagrams for such parameters as time series and the daily cycle of the pollutant concentration in selected densely populated cities. The simulation results are presented for the territory of Kazakhstan and Northern European countries.

2. Methodology

The described approach can be applied at multi-scales with downscaling modeling with NWP-ACT (Numerical Weather Prediction - Atmospheric Chemical Transport) models running at various, including high resolutions. Approach can be used to study impact of land-cover and land-use on the local and regional scale climatic conditions, e.g. temperature regime, precipitation patterns, wind characteristics, and different chemical species transport. Methodology employs online integrated meteorology-chemistry/aerosols Enviro-HIRLAM (Environment – HIgh Resolution Limited Area Model) model, Quantum Geographical Information Systems (QGIS) software package and Python programming language with visualization library Matplotlib. The Enviro-HIRLAM model is used to simulate meteorological and chemical conditions. The QGIS tool is used to process relevant (from local to regional scale) land-use and other databases and to integrate modified Enviro-HIRLAM model output in order to further perform risk assessment. Python is used for linking modelling results and GIS, through extracting data from model output files as well as visualization of meteorological and chemical fields.

2.1. EcoRisk Assessment System

2.1.1. Background information

The paper describes the RANDOM (Risk Assessment of Nature Detriment due to Oil spill Migration) system that supports the web-access to the scientifically justified risk-model. Specifically, the model designed to assess the negative impact on the marine biological environments during possible emergency oil spills in the shallow waters of the North Caspian Sea. The RANDOM system is oriented on professional users from the exploration, development and exploitation of oil fields in the North Caspian shelf. The main segments/ blocks of the user interface of the system are given at the Figure 1.

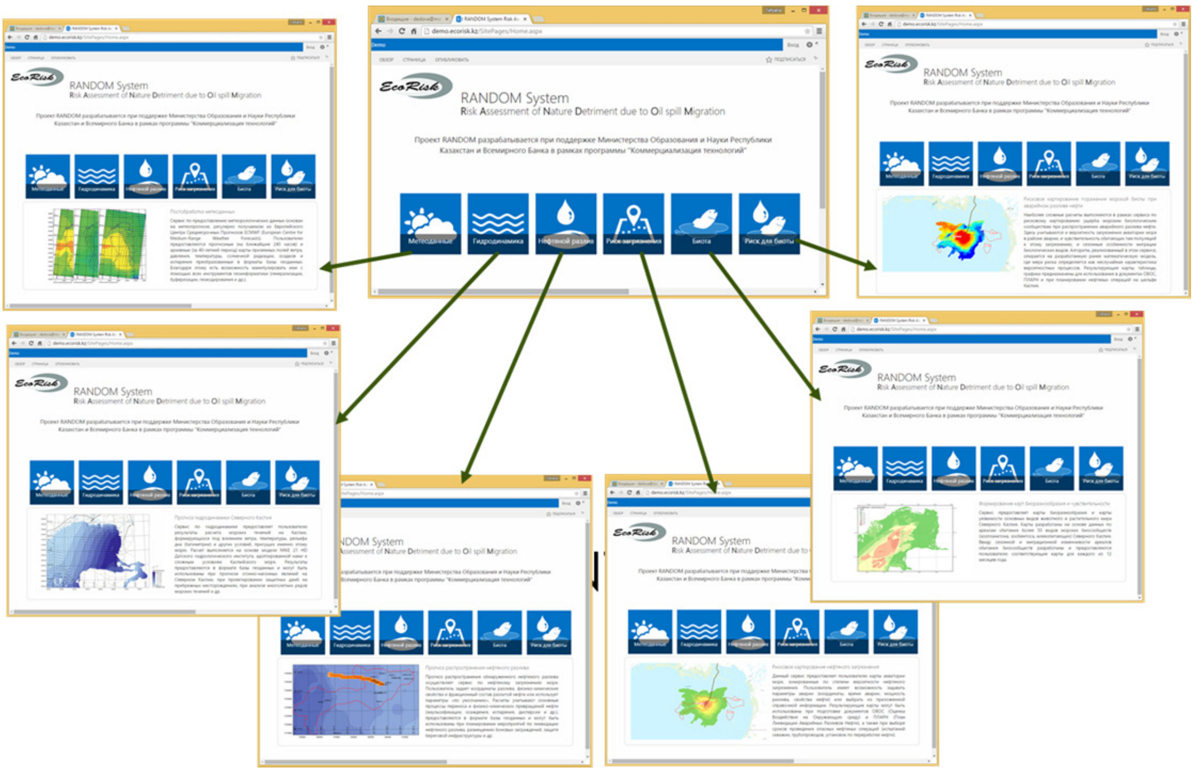


Figure 1. Main segments/ blocks of the user interface of the RANDOM system.

2.1.2. Basic components/ services

The following main basic services are developed in the RANDOM system:
1. Post-processing of the meteorological data;
2. Forecast of the hydrodynamics of the North Caspian Sea region;
3. Forecast of the oil spill distribution;
4. Risk mapping of the oil pollution;
5. Risk mapping of the marine biota's affection.

The "Post-Processed Meteorological Data" service is based on the forecast, regularly received from the European Centre for Medium-Range Weather Forecasts (ECMWF). The user is given the forecast (up to the next 120 hours), data of surface wind fields, pressure, air and sea surface temperatures, converted to digital and vector formats. Thanks to the latter that it is possible to manipulate with them using the tools of GIS.

The "North Caspian Sea Hydrodynamics Forecast" service provides the user with results of the calculation of sea currents in the Caspian Sea, formed by wind, bottom topography (bathymetry) and other conditions that are inherent to this sea. The calculation is performed in the module MIKE 21 Hydrodynamic (HD) of Danish Hydrological Institute (DHI), which is adapted by us to specific conditions of the Caspian Sea.

The "Forecast of Oil Spill" is the service for the calculation of the distribution of the oil spill, working in real time; and it provides the user with the maps of the distribution of the oil slick over the sea surface from the sources specified by the user, and taking into account the entered physico-chemical properties of the oil. The calculations are carried out employing the MIKE-21 Oil Spill model, which takes into account the basic processes of transfer and physical-chemical transformations of oil (emulsification, precipitation, evaporation, dispersion, dissolution, biodegradation, etc.). Results are available in vector format and can be used in planning for oil spill response, placing booms, protection of coastal infrastructure and others.

The "Risk Mapping of Oil Pollution" service carries out the construction of the oil marine pollution risk maps. Map zoned by the degree of probability of oil pollution. The resulting maps can be used in the preparation of documents EIA (Environmental Impact Assessment) and POS (Plan Oil Spill), as well as in choosing the timing of the hazardous oil operations (test wells, pipelines, oil refine installations).

The "Risk Mapping of the Negative Impact on the Biota" service performs mapping of risk of damage to marine biological communities with the propagation of oil spills. This takes into account the probability of sea pollution in vicinity of the accident, and the sensitivity of the population living there to this contamination, and especially seasonal migration of species. The resulting maps and charts are designed for use in EIA documents, POS and planning of oil operations on the Caspian Sea shelf.

So, as an additional service for the evaluation and analysis of atmospheric pollution it is planned to use the model Enviro-HIRLAM.

2.2. Enviro-HIRLAM: Environment – HIgh Resolution Limited Area Model

2.2.1. General description

The Enviro-HIRLAM is a fully online integrated numerical weather prediction (NWP) and atmospheric chemical transport model (ACTM) system, used for forecasting and research of meteorological and chemical weather (Baklanov and Korsholm, 2008; Baklanov et al., 2008). The meteorological and chemistry model uses equations describing six processes: emission, advection, horizontal diffusion, vertical diffusion and dry deposition, convection and wet deposition, chemistry and aerosols (Korsholm et al., 2008). The system realization includes six main steps which are the following: nesting of models for higher resolutions, improved resolving of boundary and surface layers characteristics and structures, different levels of urbanization, improvement of advection schemes, implementation of chemical mechanisms, implementation of aerosol dynamics, realization of feedback mechanisms, and assimilation of monitoring data (Baklanov et al., 2008).

2.2.2. Domains of interests

Before starting the calculation, the model domains should be defined. Defining and setting up new modelling domains is initial preparatory step to further calculate the climate generation files for a chosen resolution. Three modeling domains – K15, CA5, and S15 – varying in geographical extension and resolution, were created for the project. All domains are constructed in the rotated system of coordinates (RSC). RSC is used to keep the size of domain grid cells almost equal. The parameters of these domains extents are given Table 1.

Table 1. Model domains parameters for Enviro-HIRLAM-K15, -CA5, and -S15 domains.

Description of parameter	**Parameter**	**K15**	**CA5**	**S15**
Horizontal resolution in degrees	RES	0.15	0.05	0.15
Horizontal resolution in km		15	5	15
Domain size				
Number of grid points along longitude	NLON	334	410	460
Number of grid points along latitude	NLAT	148	270	300
Number of vertical levels	NLEV	40	40	40
Width of boundary zone	NBNDRY	10	10	10
Total number of grid points in the domain		49432	110700	138000
Area covered by the domain in km^2		11122200	2767500	31050000
Domain boundaries (in RSC)				
South border	SOUTH	25,495	30,000	26,500
North border	NORTH	47,545	43,450	71,350
West border	WEST	0,495	7,550	-10,150
East border	EAST	50,445	28,000	58,700
Pole latitute	POLAT	-80,0	-80,0	-80,0
Pole longitude	POLON	30,0	30,0	0,0

For territory of Kazakhstan, the modeling domain with 0.15° horizontal resolution (334 x 148 grid points along longitude and latitude, correspondingly) has been chosen. The domain is represented with the following pole coordinates: PoLon = 30°, PoLat = -80° and the coordinates of domain boundaries at: south = 25.495, north = 47.545, west = 0.495, and east = 50.445 degrees. The domain covers the whole territory of Kazakhstan as well as the territories of neighboring countries. The covered domain area is shown in Figure 2. In order to obtain results with a better horizontal resolution it is necessary to carry out the calculation using both the initial and boundary conditions of the previous simulation runs. After obtaining the results of the run for the K15 domain (with about 15 km resolution), using these data we will be able to run the simulation at 5 km resolution.

To achieve this, we need to define a domain region CA5 placed within boundaries of the existing domain K15 (see Figure 2) and having a set of parameters given in Table 1.

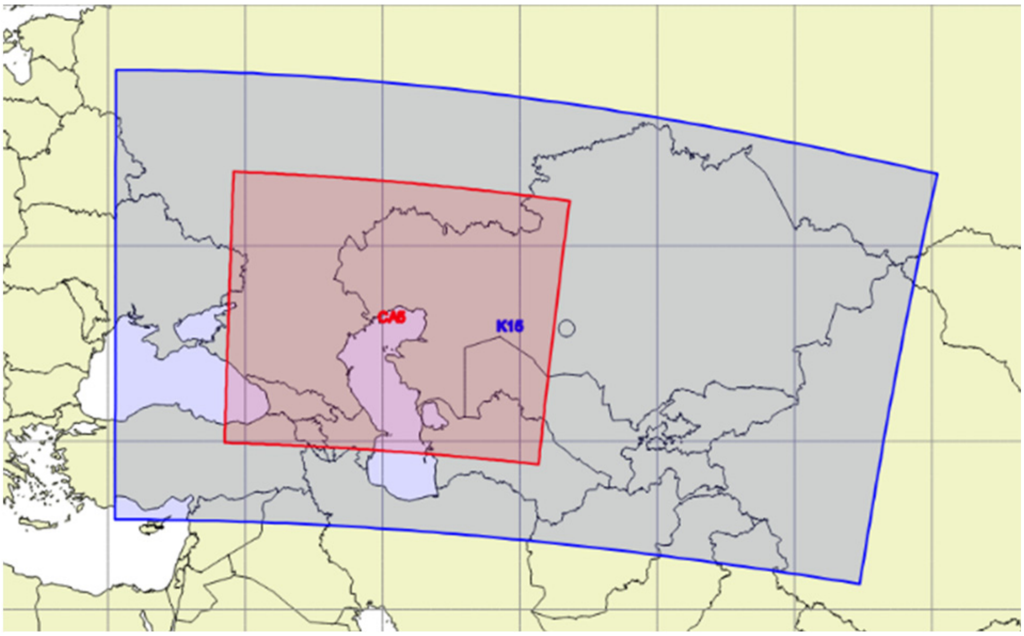


Figure 2. Enviro-HIRLAM-K15 (blue) and -CA5 (red) Kazakhstan domains with resolutions of 0.15 and 0.05 [degrees], respectively.

For the territory of Europe the domain with a horizontal resolution of 15 km (or 0.15 degrees) was also selected. The obtained calculation area is 460 x 300 grid cells. Domain is defined in the rotated coordinate system, so the pole selected as follows: PoLat = -80.0, PoLon = 0. The coordinates of domain boundaries at: south = 26.500, north = 71.350, west = -10.150, and east = 58.700. The domain S15 covers the whole of Europe territory and part of western Asia area. The covered area is shown at Figure 3 and the required parameters are also given in Table 1.

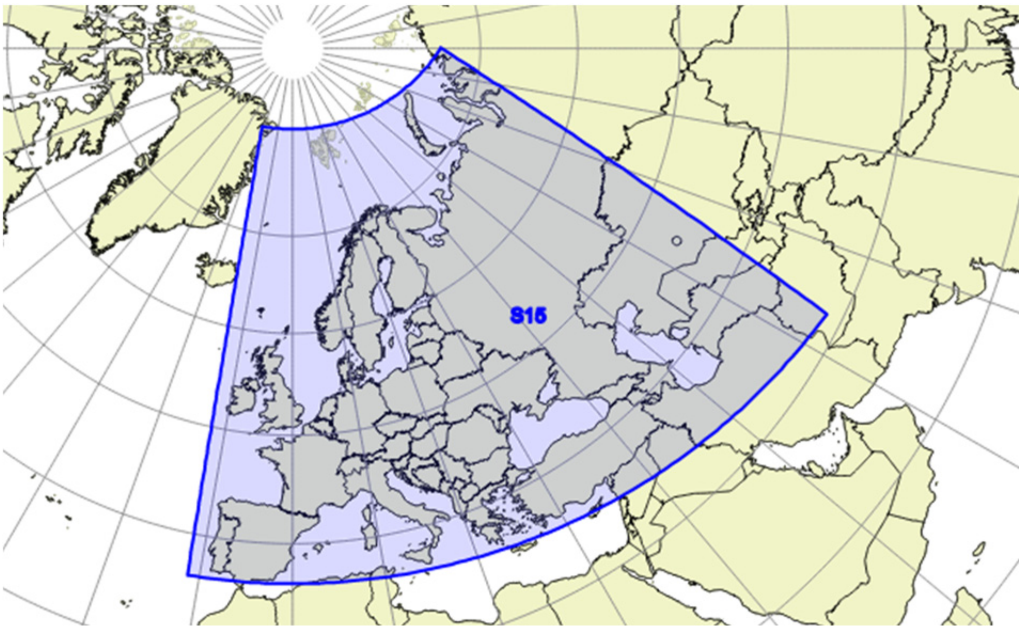


Figure 3. Enviro-HIRLAM-S15 (blue) Europe domain with resolution of 0.15 [degrees].

2.2.3. Initial and boundary conditions for meteorology and chemistry

Meteorological initial and boundary conditions (IC/BCs) had been retrieved from ECMWF-IFS model (European Centre for Medium-Range Weather Forecasts - Integrated Forecasting System) (http://ecmwf.int) with horizontal resolution 0.75°. These data are global in coverage and include initial and boundary fields for such meteorological parameters as the air temperature, wind speed, specific humidity, and surface pressure. The retrieved IC/BC dataset covers period from 16 till 27 January 2010 inclusive and has 3-hour temporal resolution.

The MACC (Monitoring Atmospheric Composition & Climate; Melas et al., 2014) retrospective analysis (reanalysis) data were used as chemical IC/BCs in the frame of the project. The global coverage data were downloaded from the ECMWF Data Server (http://apps.ecmwf.int/datasets/data/macc-reanalysis) with 1.125° horizontal resolution for the same period as meteorological IC/BCs and with the same temporal resolution. The following gases and aerosol species were extracted from the MACC dataset and used in the Enviro-HIRLAM simulations: black carbon (BC) and organic matter (OM) of both hydrophilic and hydrophobic types, dust for three different size ranges (0.03–0.55, 0.55–0.9, and 0.9–20 μm), ozone (O_3), sulphate and sulphur dioxide (SO_2).

The emission inventory ECLIPSE v5a (Evaluating the Climate and Air Quality Impacts of Short-Lived Pollutants; see more detailed description of the emission inventory at *http://www.iiasa.ac.at/web/home/research/researchPrograms/air/ECLIPSEv5a.html*) with anthropogenic emissions was used in the study as well. The data were created with the GAINS (Greenhouse gas – Air pollution Interactions and Synergies) model providing emissions for both long-lived greenhouse gases and short-lived aerosol species (http://gains.iiasa.ac.at). The ECLIPSE v5a data are global in coverage with 0.5° horizontal resolution and represented by accumulated amount of air pollutant per year (i.e. in kt/year) in each grid cell.

The following chemical species from the emission inventory have been used in the Enviro-HIRLAM: BC, OM and SO_2. For each pollutant, the emission data correspond to so-called 10 SNAP (Standard Nomenclature for Air Pollution) codes, which are corresponding to various emission sectors (see Table 2). For our simulation scenario the SNAP-3 (combustion in manufacturing industry) was selected.

Table 2. Standard Nomenclature for Air Pollution (SNAP) emission sectors.

№	**SNAP code**	**Sector**
1	SNAP-1	Combustion in energy and transformation industries
2	SNAP-2	Non-industrial combustion plants
3	SNAP-3	Combustion in manufacturing industry
4	SNAP-4	Production processes
5	SNAP-5	Extraction and distribution of fossil fuels and geothermal energy
6	SNAP-6	Solvents and other product use
7	SNAP-7	Road transport
8	SNAP-8	Other mobile sources and machinery
9	SNAP-9	Waste treatment and disposal
10	SNAP-10	Agriculture

2.3. Sources of Emissions and Scenarios

2.3.1. Accidental release at oil storage facility

In Kazakhstan, oil refining generally develops simultaneously with the increase in oil production. Currently, there are 3 major oil refineries with total refining capacity of nearly 19.5 million tons. Oil refining industry of Kazakhstan is represented by three large enterprises - LLP "Atyrau Oil Refinery", LLP "Pavlodar Petrochemical Plant" and LLP "PetroKazakhstan Oil Products" (previously – Joint Stock Company (JSC) "ShymkentNefteOrgSintez") (Tables 3 and 4).

Table 3. Major enterprises of the oil refining industry of Kazakhstan.

Oil Refineries	Controlling shareholder	Refining capacity (million tones)	Refining depth, (%)	Region	Commis sioning date
LLP "Atyrau Oil Refinery"	KazMunaiGas	5.2	83	Atyrau region	1945
LLP "Pavlodar Petrochemical Plant"	KazMunaiGas	8.0	85	Pavlodar Region	1978
LLP "PetroKazakhstan Oil Products"	PetroKazakhstan	6.2	62 (2007)	South Kazakhstan Region	1984

Table 4. Geographical coordinates of the oil refineries.

Oil refinery	Latitude (°N)	Longitude (°E)
LLP "Atyrau Oil Refinery",	47.0734	51.9261
LLP "Pavlodar Petrochemical Plant"	52.3697	76.9082
LLP "PetroKazakhstan Oil Products"	52.3697	76.9082

For the experiment simulation of the distribution of sulfur dioxide (SO_2) during emergency emission in Kazakhstan, we have chosen the Atyrau oil refinery, located in the city of Atyrau (Republic of Kazakhstan). This plant, located near the Caspian Sea, is one of three major refineries in Kazakhstan (Figure 4). Atyrau refinery is the firstborn refinery in Kazakhstan. The plant was put into operation on September 8, 1945. The first product of the plant was gasoline. Since mid-1999, the holder of a controlling stake (86%) of the plant was CJSC "KazakhOil", subsequently - JSC "KazMunaiGas".

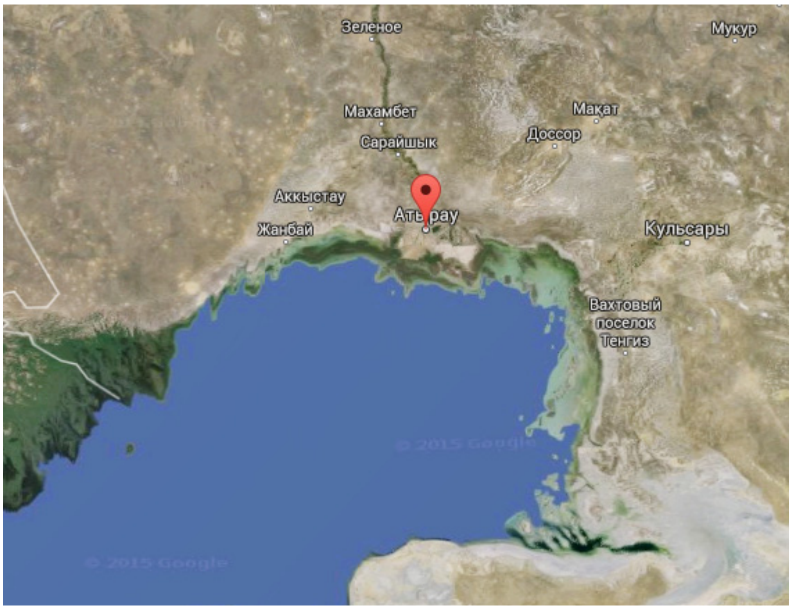


Figure 4. Geographical location of the Atyrau oil refinery.

During the combustion of petroleum products a huge amount of toxic mixture is released into the atmosphere. For the high-sulfur oil a predominant role in the pollution plays the sulfur dioxide (SO_2). The main purpose of this study is to analyse atmospheric transport and deposition of pollutants in case of the emergency accidental release from the Atyrau oil refinery, as well as the assessment of its impact on the territory of Kazakhstan and the neighboring countries.

2.3.2. Continuous emissions from smelters of metallurgical enterprises

For the experiment simulation of the distribution of sulfur dioxide (SO_2) in relation to continuous emissions several plants of the JSC "Kola MMC" located in the Kola Peninsula were chosen. The JSC "Kola Mining and Metallurgical Company" (JSC "Kola MMC") is a subsidiary of PJSC MMC "Norilsk Nickel" is the leading manufacturing complex of the Murmansk region (Russia), created on the basis of the oldest enterprises of Severonikel and Pechenganikel, is a single-mining for the extraction of copper-nickel sulfide ores and the production of non-ferrous metals.

The founders of the Kola MMC were two subsidiaries of the Open Joint Stock Company "Russian Joint Stock Company for the production of non-ferrous and precious metals" Norilsk Nickel" (OJSC" RJS "Norilsk Nickel") located on the Kola Peninsula: OJSC " Pechenganikel Mining and Metallurgical Combine" and JSC "Severonikel Combine." Those are the oldest enterprises of the Murmansk region, carrying out their activity from 1930-40-ies.

Divisions of Kola Mining and Metallurgical Company are geographically distant from each other. They are located at the center of the Kola Peninsula - the city of Monchegorsk (Severonikel Combine) and at the north-west of the Murmansk region - in the Nikel and Zapolyarny cities (Pechenganikel Combine) (Figure 5).

Figure 5. Kola Mining and Metallurgical Company (KMMC) factories.

2.4. Modelling Experiments

2.4.1. Selected meteorological episodes

The study is focused on the time period from 17th till 26th of January 2010. The selection of days was based on the criteria of the calm dominating conditions during the entire day. The low wind conditions (LWC) days were selected in order to minimize synoptic scale effects. The criteria for calm day are: clear sky, low wind speed (below 3 m/s), frequently shifting wind direction, lower relative humidity, high atmospheric pressure, and horizontally close to homogenous temperature field (Velazquez-Lozada et al., 2005). Simulations were performed for all days, which had Typical Wind Condition (TWC).

2.4.2. Technical setup for the control/ reference run

The results of these simulations are necessary so that after adding the source it is possible to conduct a comparative analysis, as well as to ensure that the model is working correctly for the whole selected period. The settings are shown in K15 domain example, and for the rest of the domains the program settings are identical in except for the domain parameters directly. To do this, we have to set the following program settings and run the simulation.

At first, we created the project working directory (K15) and to copy all necessary files to set up and operate the Enviro-HIRLAM model. Setup of the K15 model included required modifications for the number of grid points along latitude and longitude, number of vertical levels, boundaries (at north, south, east, and wets) of the model domain in the rotated system of coordinates, position of the pole (latitude and longitude), number of passive boundary points, width of the boundary zone, as well as number of halo-zone points, dynamical time step, climate data set projection as well as its resolution, frequency of the output results, link to the boundary conditions taken from ECMWF (or Enviro-HIRLAM model domains). At second, paths and switches to modules and meteorological boundary conditions to be used were activated as well as paths to emission inventories files. At third, for emission inventories the scaling factors were introduced for applied datasets.

After all have been prepared the launch run of the model can be initiated, where it is necessary to specify the beginning and end of the simulation period as well as forecast time period. In our study the forecast was restarted with new boundary conditions at every 6 hour time interval indicated.

2.4.3. Run with accidental release

To add a source of pollution in our calculations, we need to know the source's location, release date, duration of release and the rate of emission of the analyzed chemical species (in this case is SO_2). As it was mentioned above, we have chosen the source of contamination as the Atyrau refinery, and will evaluate the air pollution with sulfur dioxide (SO_2), which is a strong toxic substance. Coordinates of source are known, the release is assumed to last during 24 hour time interval, and so, it remains to determine the rate of pollutant emissions.

We define a scenario in which the emergency occurred and a fire started in an oil reservoir with a volume of 5000 m^3. Assume that the combustion of petroleum products occurs all over the tank top surface. The height of the cylindrical reservoir is about 11.9 meters, which means that the surface of the reservoir area is 420 m^2 (http://worldtek.ru/neftegaz/291-osnovi-nefteaza-hranenie-nefti-transport-gaza.html?showall=1). When burned, petroleum product with an area of 1 m^2, there is sulfur dioxide released in the amount of 405 kg per hour (http://response.restoration.noaa.gov/oil-and-chemical-spills/oil-spills/resources/in-situ-burn-emissions-comparisons.html). As a result, when the reservoir ignition the SO_2 emission rate is 170 100 kg per hour. For our case, we simulate a situation, where the emission duration is 24 hour and we will have about 4082.4 tonnes of sulfur dioxide released into the atmosphere.

As a summary of above analysis, for the simulation of accidental scenario for simultaneous numerical weather forecast and atmospheric transport of pollution on the territory of Kazakhstan the following options were chosen:

1) Release date is January 20, 2010. Duration of simulation is 5 days after the end of emission. The initial and boundary conditions for the simulation are selected for January 16 to January 26, 2010, and so. the chemical data from January 17, 00 UTC to January 26, 00 UTC 2010. Thus, the Enviro-HIRLAM model is launching to run from January 17 to January 26, 2010.
2) Emission source (point source) is the Atyrau Oil Refinery (latitude: 47.0734°N, longitude: 51.9261°E).
3) Release rate is 170100 kg per hour.
4) Emission duration is 24 hour.
5) Pollutant substance considered is sulfur dioxide (SO_2).

Necessary modifications were made in the model code in order to set the continuous and point emission sources coordinates and release of emissions. Similarly to the control/ reference run, the beginning and end of the simulation period as well as forecast time period were specified before the model run.

2.4.4. Run with continuous emission

To add the pollution sources in the case of continuous emission, we need to know the coordinates of the source and chemical species to be analyzed. As mentioned above, as the source of contamination we have chosen the Kola MMC, and will evaluate the air pollution with sulfur dioxide (SO_2) emissions in case of double increasing of the existing emission. The rate of SO_2 emission from each selected source is about 30 thousand tonnes per year. Let us define a scenario in which the rate of SO_2 emission from each selected source is 60 thousand tons per year. As a result, for the simulation of numerical weather forecast and pollution atmospheric transport for the Northern European domain, we have selected the following options:

1) Simulation period - from January 17 to January 26, 2010.

2) Emission sources - Pechenganikel plant in the city of Nickel (latitude: 69.4140°N, longitude: 30.2367°E) and city of Zapolyarny (latitude: 69.4068°N, longitude: 30.7975°E) and Severonikel plant in the city of Monchegorsk (latitude: 67.9111°N, longitude: 32.8385°E).

3) The total release is 60000 tonnes per year.

4) Duration of the release – continuous (i.e. during all simulation period considered)

5) Pollutant substance - sulfur dioxide (SO_2).

Similarly to the accidental release scenario, all necessary modifications were made in the model code in order to set the continuous emission sources coordinates and release of emissions. Similarly to the control/ reference run, the beginning and end of the simulation period as well as forecast time period were specified before the model run.

2.4.5. Run with scaling for the finer resolution

To obtain the results with finer horizontal resolution it is necessary to launch the calculation for the new Enviro-HIRLAM - CA5domain located inside the given K15 domain, but with about 3 times less area. To accomplish this we adjusted a number of model parameters and settings. N particular, number of grid points along latitude and longitude, boundaries (at north, south, east, and wets) of the model domain, number of passive boundary points, width of the boundary zone, as well as number of halo-zone points, dynamical time step (from 240 to 120 sec), link to the boundary conditions taken from Enviro-HIRLAM-K15 model. At second, paths and switches to modules and meteorological boundary conditions to be used were activated as well as paths to emission inventories files, boundary strategy from "operational" to "same_cycle", activated option "nesting" and changed boundaries interval from 6 to 3 hour. At third, for emission inventories the scaling factors were introduced for applied datasets as resolution of Enviro-HIRLAM model domain was changed from 15 to 5 km.

Similarly to the previously described runs and scenario, all necessary modifications were made in the model code in order to set the continuous emission sources coordinates and release of emissions, and similarly, the beginning and end of the simulation period as well as forecast time period were specified before the model run.

2.5. Approaches to Visualization and Data Analysis

2.5.1. Model output

The forecast model writes its primary output to the GRIB-format binary type file (fcyyyymmdd_hh+lll), which is designed to be a complete snapshot of the model state described by the NWP HIRLAM model for a particular time point (on the hour). In addition, through specification of the namelist NAMPPP, more model output including post-processing/ diagnostic fields can be written out during the forecast model integration, such as those model diagnostics (with suffix *md such as fcyyyymmdd_hh+lllmd), pressure and single level parameters for field verification and observation verification (with suffix *ve such as fcyyyymmdd_hh+lllve). In the tables below, abbreviations used for the different file type are: fc=history file, fcmd=diagnostics file and fcve=verification file.

2.5.2. Post-processing and interpolation approaches

For subsequent processing of generated output files, the Python programming language was used with accession to libraries such as *pygrib* – for reading, processing, and recording of GRIB-format files, *matplotlib* – for data visualization and *numpy* – basic package for scientific computing and efficient multi-dimensional analysis and storage of generic data. In our study, we analyzed the concentrations of sulfur dioxide (SO_2) in selected Kazakhstan's cities (having population over 50 thousand inhabitants) and the capitals of the European countries and cities with a population of over a million people. The period considered is from January 17 till January 26, 2010. Since the horizontal resolution of the simulation is 15 km; so, for the accuracy of determining the value at a point, we interpolated the data around the study area. Interpolation was held only near the point, to reduce the run time and engaged memory, affected in the calculation. To achieve this, 4 types of interpolation were used: average for nearest neighbor (average), linear (linear), cubic spline (cubic) spline of 5th order (quintic) (see Figure 6). As a result, the average of these 4 interpolation methods was chosen. Figures 7 and 8 you show the results of the data interpolation around the selected cities of Kazakhstan and Europe (on date of 21st Jan 2010, 08 UTC).

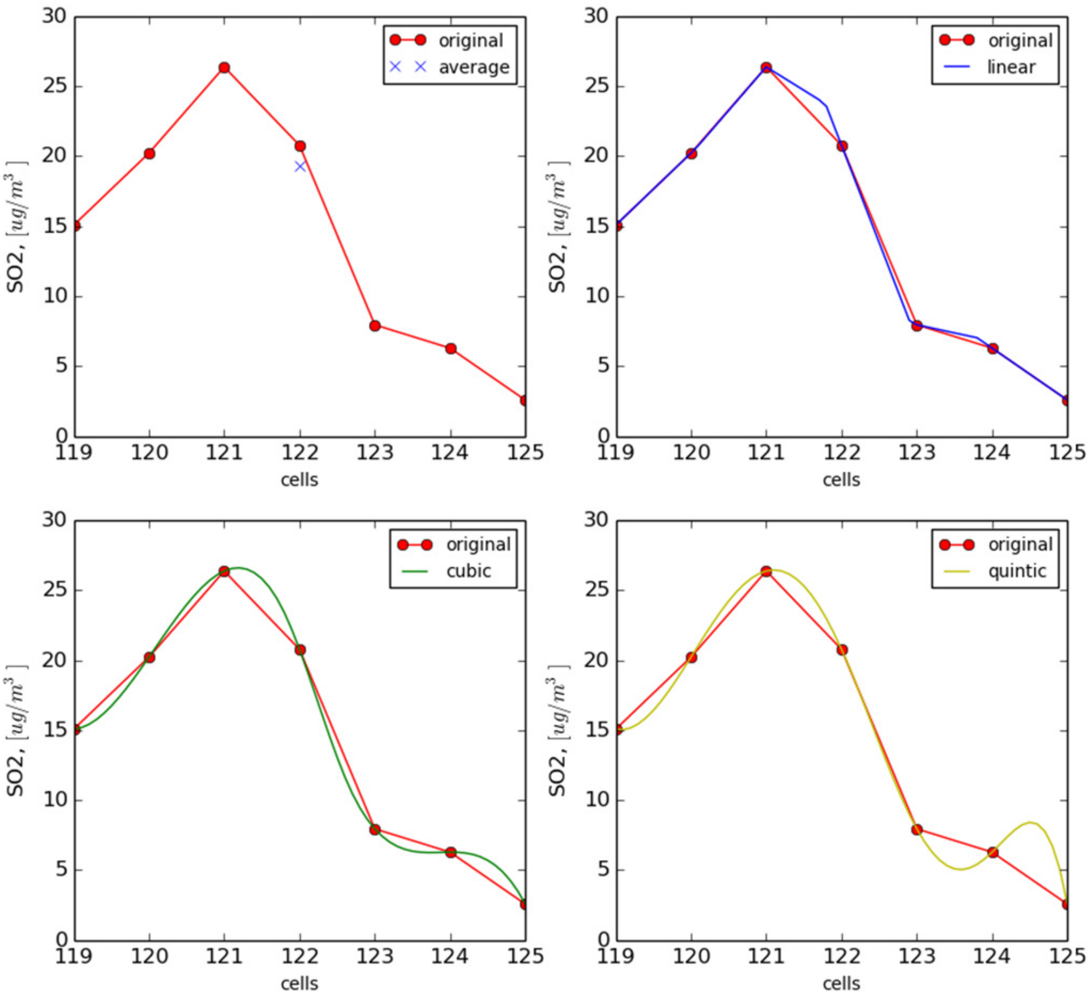


Figure 6. Examples of interpolation of SO_2 concentrations [$\mu g/m^3$] using different methods.

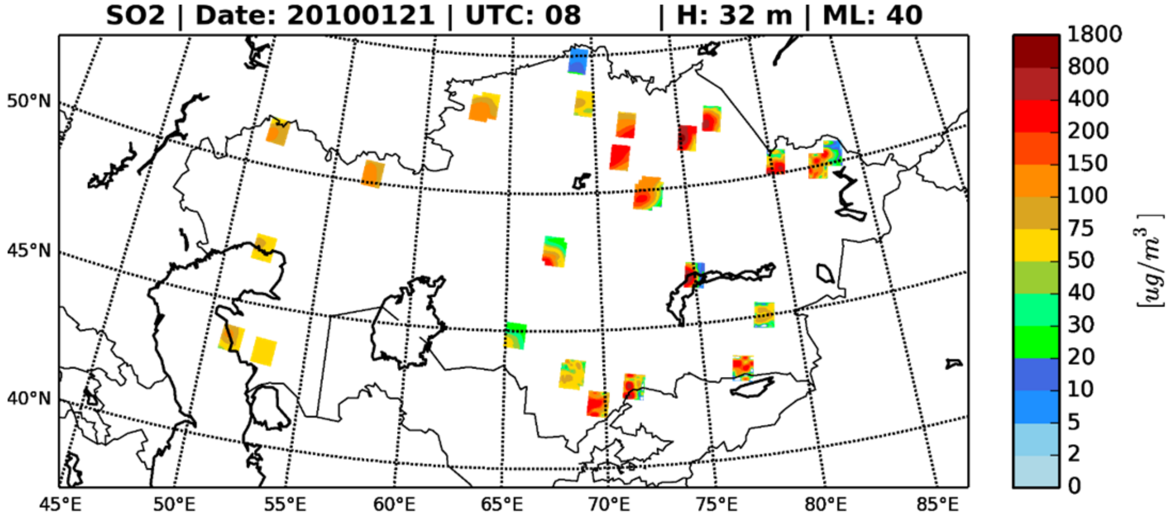


Figure 7. Interpolated data of SO_2 concentrations for the selected cities of Kazakhstan.

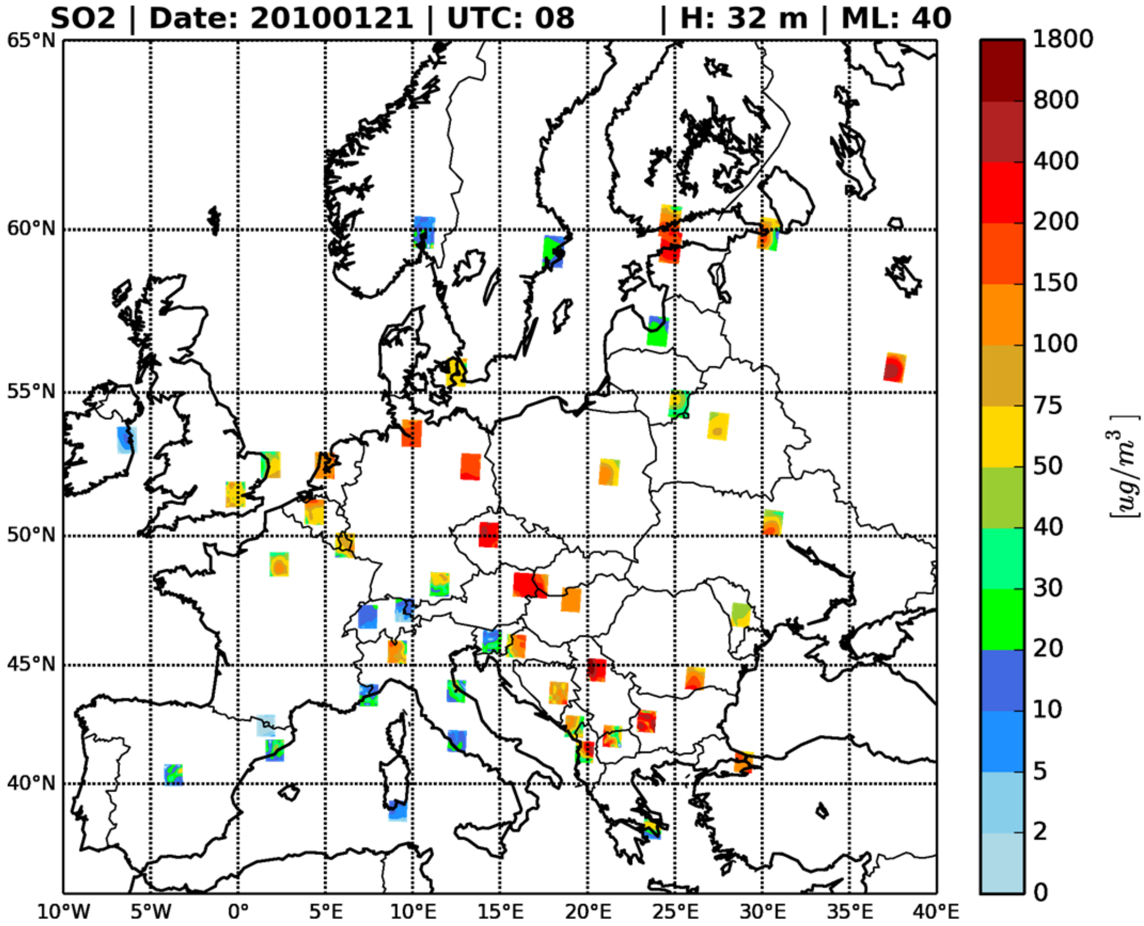


Figure 8. Interpolated data of SO_2 concentrations for the selected cities of Europe.

2.5.3. Spatio-temporal variability, time-series, and diurnal cycle

Using developed program in Python, the spatio-temporal variability of concentrations of SO_2 was obtained as well as meteorological fields such as wind, air temperature, humidity, pressure, etc. The obtained results are presented as a series of 2D maps, which have been assembled into a single animated GIF-format file (for each parameter). The time-series covering period from January 17 to

January 26 for the cities of Kazakhstan and Europe was built and analyzed. Moreover, the daily cycles (averaged over 9 day period of modeling) were built too. Thereby, the data of meteorological and chemical fields simulation results were analyzed.

2.5.4. GIS integration of modelling results

Visualization and analysis of the results obtained with the use of the Enviro-HIRLAM model were performed in a GIS environment. The effect of sulfur dioxide from the accidental release from the Atyrau refinery on the population of nearby regions has been analyzed. To solve this problem we have used the QGIS (http://www.qgis.org/en/site) means that provides a wide range of tools for processing simulation results. The output files created by the model Enviro-HIRLAM are recorded as GRIB-format files. Beause this format is not directly supported by any GIS software, it is needed to undertake several steps to integrate the results of modelling into GIS environment. To determine and visualize the SO_2 effect on the population the following procedures were carried out:

1) Export data from the output GRIB-format files into XYZ ascii text files;
2) Import XYZ files into QGIS;
3) Convert results into data matrix (grids) with defining a geographical projection;
4) Calculate the average sulfur dioxide concentration at each point within three days from the start of emission;
5) Combine the resulting map of concentration of SO_2 with the population density map;
6) Normalize the obtained values from 0 to 100% for the evaluation of the impact on population;
7) Classify and plot the map with the appropriate scaling in legend.

3. Results and Discussions

3.1. Spatio-temporal Variability of Meteorological and Chemical Patterns in Modelling Domains

After the Enviro-HIRLAM-K15 runs were complete, the simulation results were obtained for the territory of Kazakhstan (as shown in Figures 9-13, as examples). The figures represent 2D fileds of spatio-temporal variability - of air temperature (Figure 9), atmospheric pressure (Figure 10), specific humidity (Figure 11), wind characteristics – speed and direction (Figure 12), and the concentration of sulfur dioxide (SO_2) (Figure 13) - at a height of 32 meters above the Earth's surface.

The simulated meteorological parameters are well reproduced over the model domain reflecting dominating synoptic atmospheric circulation patterns in this region, showing influence of mountain regions in the southern sector of domain, underlying influence of arid regions, etc. In particular, air temperature ranges from –30°C to +5°C from north to south on the territory of Kazakhstan, by pressure fields it can be clearly seen where the mountainous terrain, specific humidity in the South higher than the North, constant wind in the western direction is seen in East Kazakhstan and in the Caspian Sea, the SO_2 concentration patterns show clearly main and dominating sources of pollution in the studied area with the focus on Kazakhstan and adjacent areas. On the annual scale, in this geographical region the dominating atmospheric transport of pollution in the western direction is clearly seen during month of January. A relatively higher levels of concentration are seen in the vicinity of the major sources such as "Balkhashtsvetmet" (formerly known as Balkhash Mining and Metallurgical Combine) is a copper-smelting combine located on the northern coast of the Lake Balkhash in Balkhash city, LLP "Pavlodar Petrochemical Plant", Zhezkazgan Mining and Metallurgical Combine is Kazakhstan's non-ferrous metallurgy, LLP

"PetroKazakhstan Oil Products" (previously - Joint Stock Company (JSC) "ShymkentNefteOrgSintez") compared with other surrounding territories.

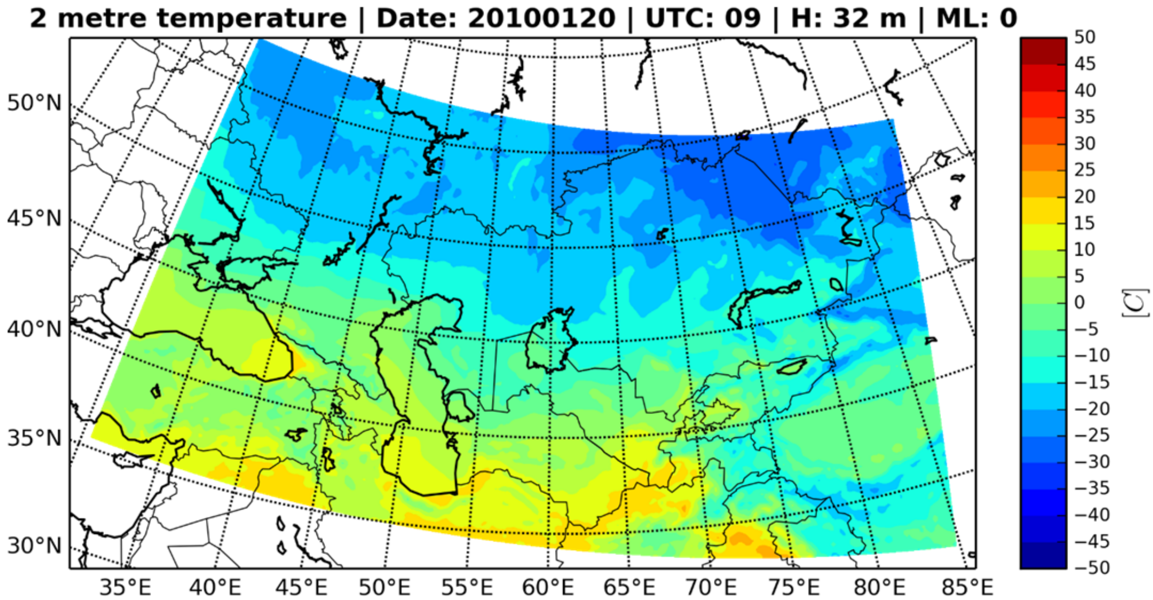


Figure 9. Temperature of the ground surface.

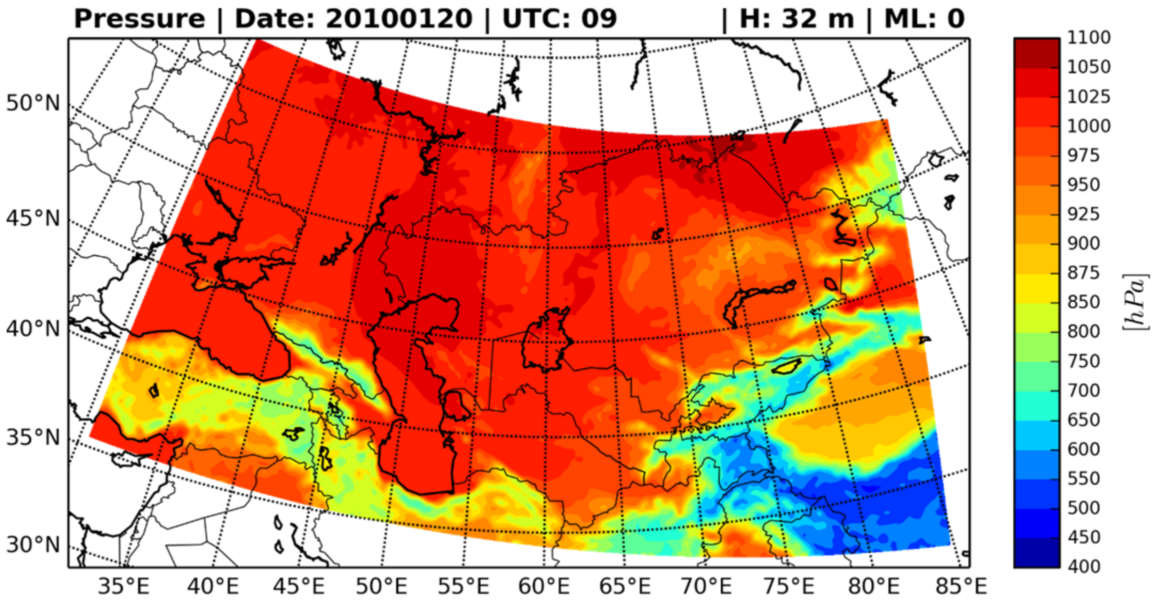


Figure 10. Pressure.

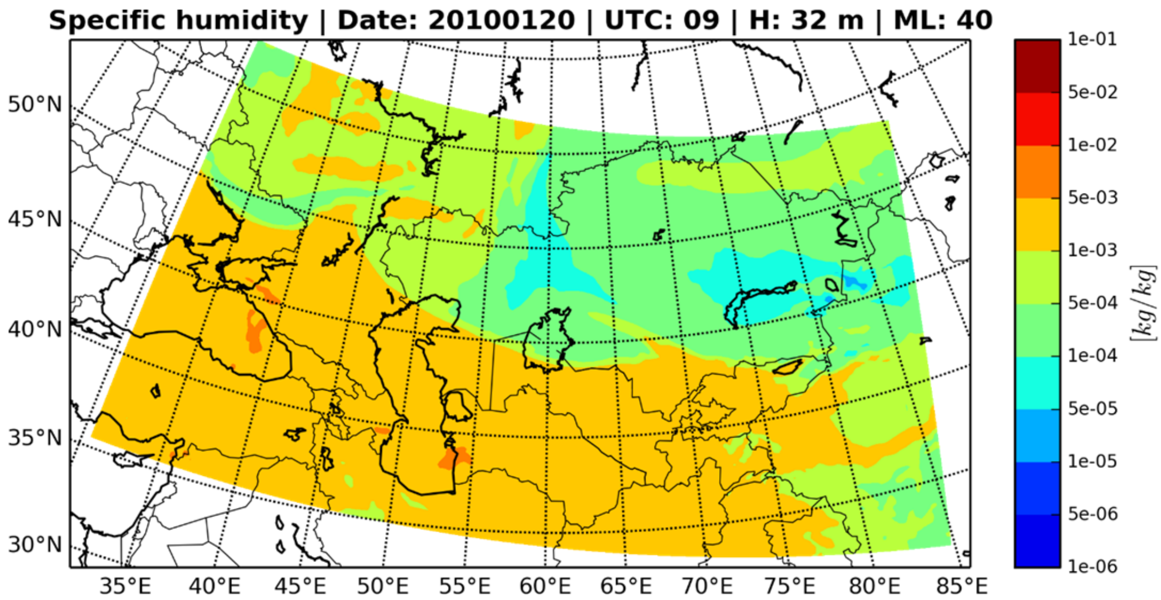


Figure 11. Specific humidity.

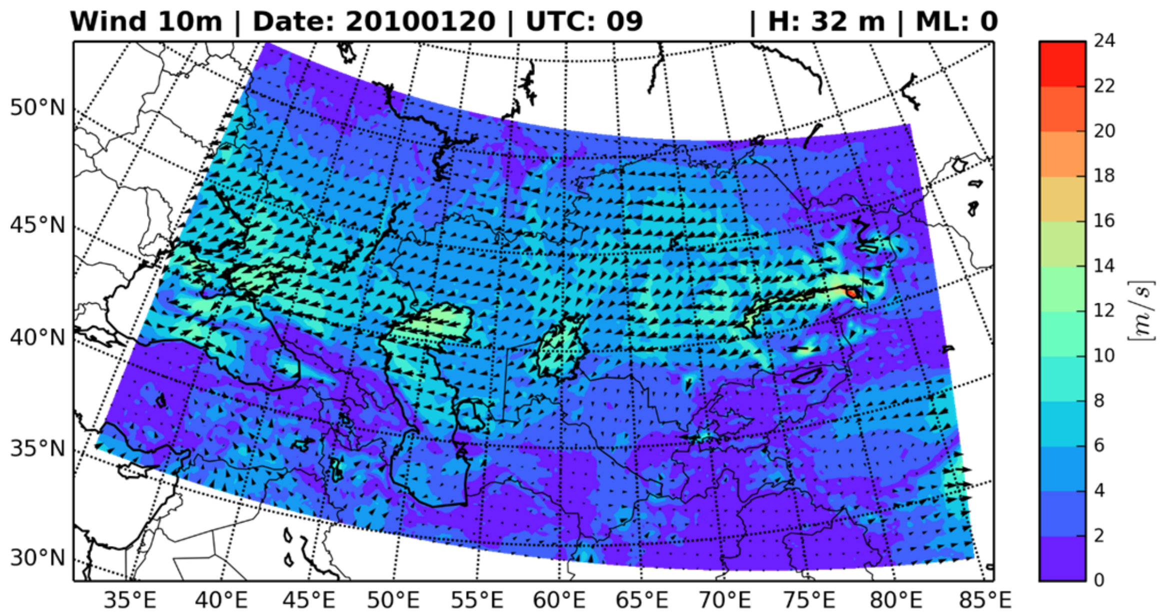


Figure 12. Wind, 10 meters above the ground surface.

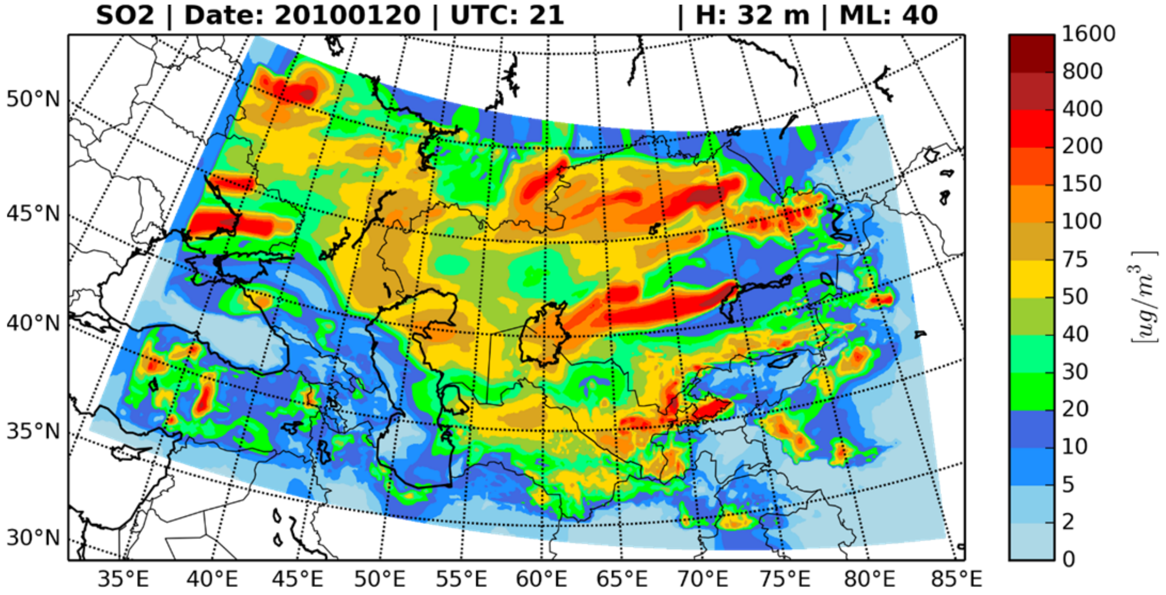


Figure 13. The concentration of sulfur dioxide (SO_2), without adding an additional source of pollution (e.g. accidental release at the Atyrau refinery).

Similarly to the Kazakhstan study, for the Northern Europe territory, the results of the Enviro-HIRLAM modeling are presented in Figures 14-18 in a form of spatio-temporal 2D fields of air temperature, atmospheric pressure, specific humidity, wind characteristics and the concentration of sulfur dioxide (SO_2) at a height of 32 meters above the surface of the Earth.

The simulated meteorological parameters are well reproduced over the model domain reflecting dominating synoptic atmospheric circulation patterns in this region, showing air temperature ranges from –25°C to +10°C from East to West on the territory of the Northern Europe, by pressure fields it can be clearly seen where the mountains in Scandinavian Peninsula, clearly seen that the sea wind is much stronger than on land, the SO_2 concentration patterns show clearly main and dominating sources of pollution in the studied area. A relatively higher levels of concentration are seen in the vicinity of the major sources such as Mining and Metallurgical Combines in Kola Peninsula, plants in Chelyabinsk, pollutants from Moscow, Saint-Petersburg, Tallin, Narva cities compared with other surrounding territories.

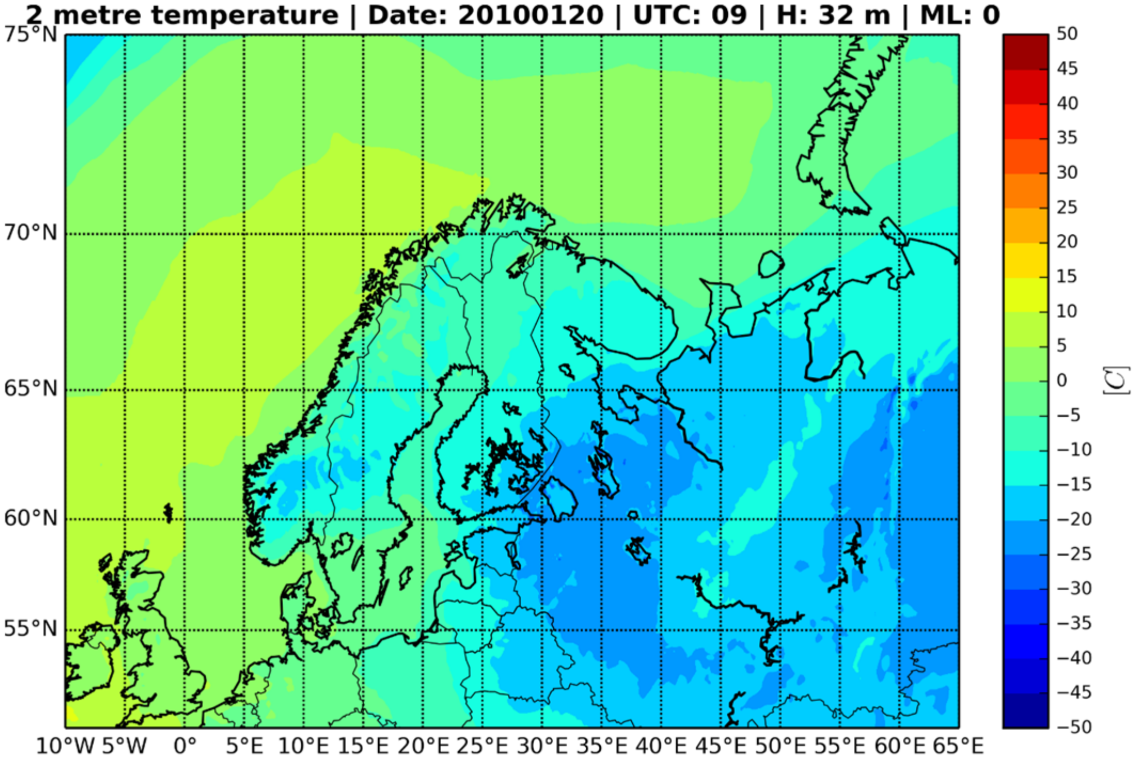


Figure 14. Temperature of the ground surface.

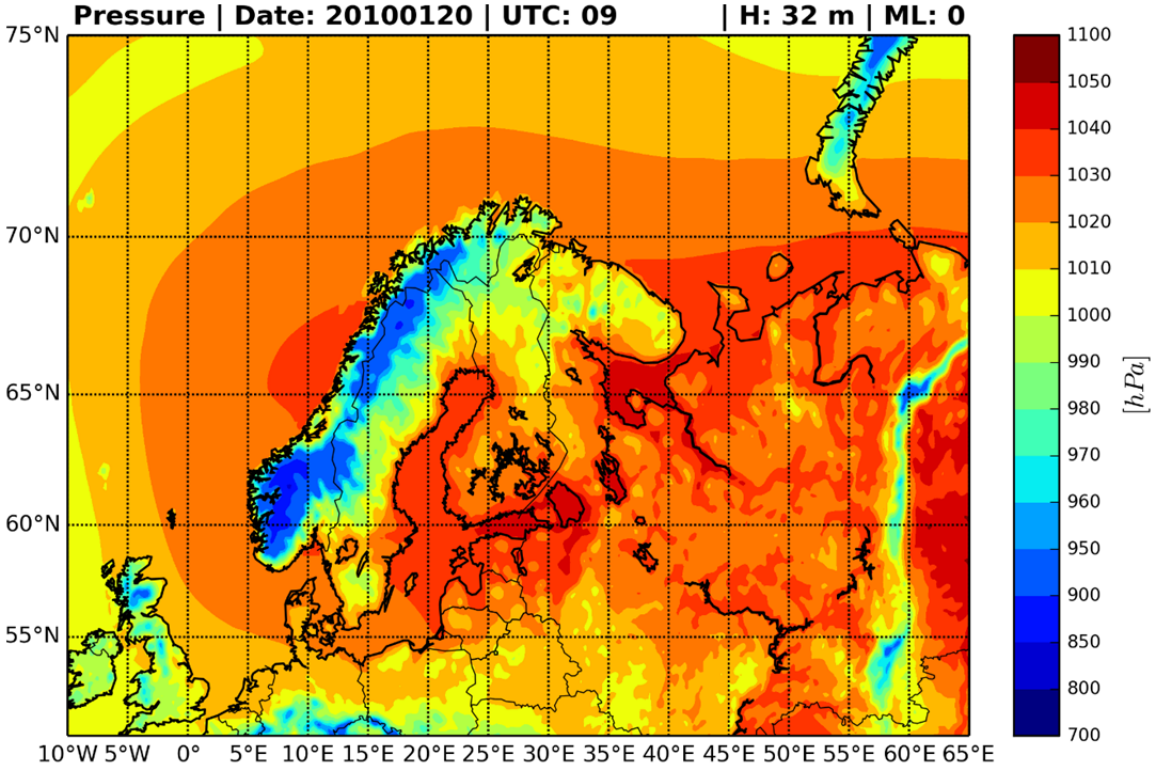


Figure 15. Pressure.

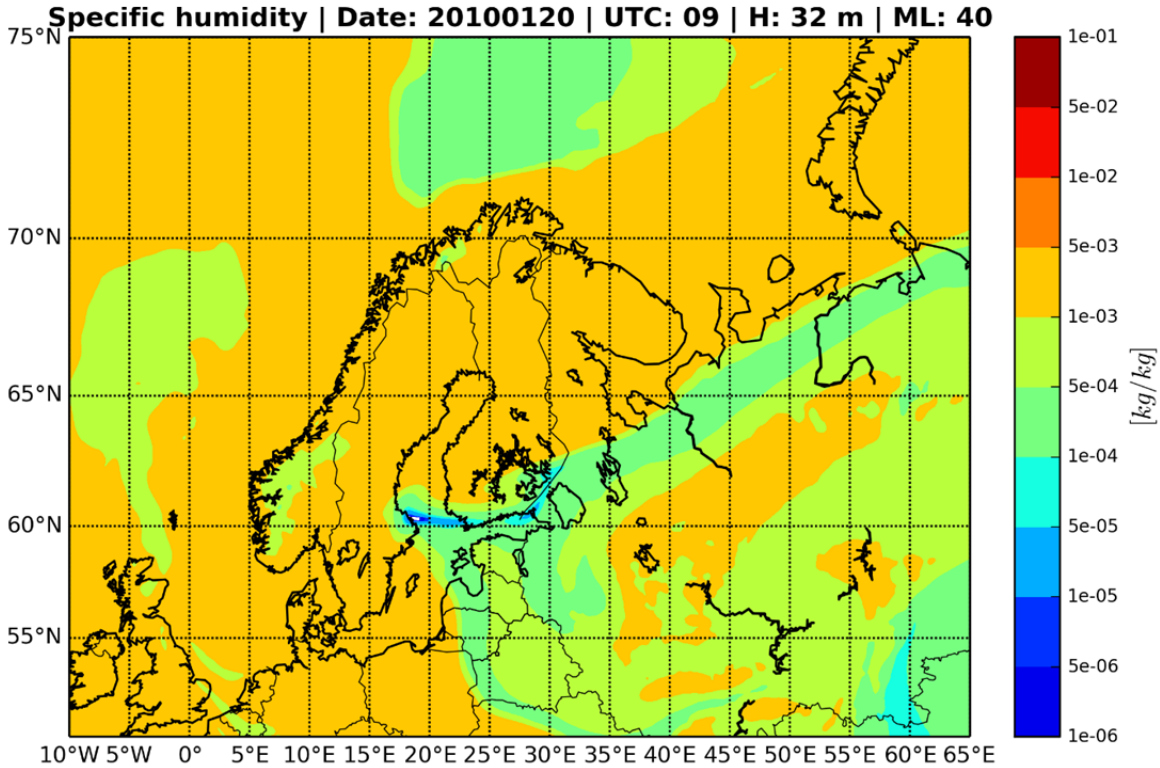


Figure 16. Specific humidity.

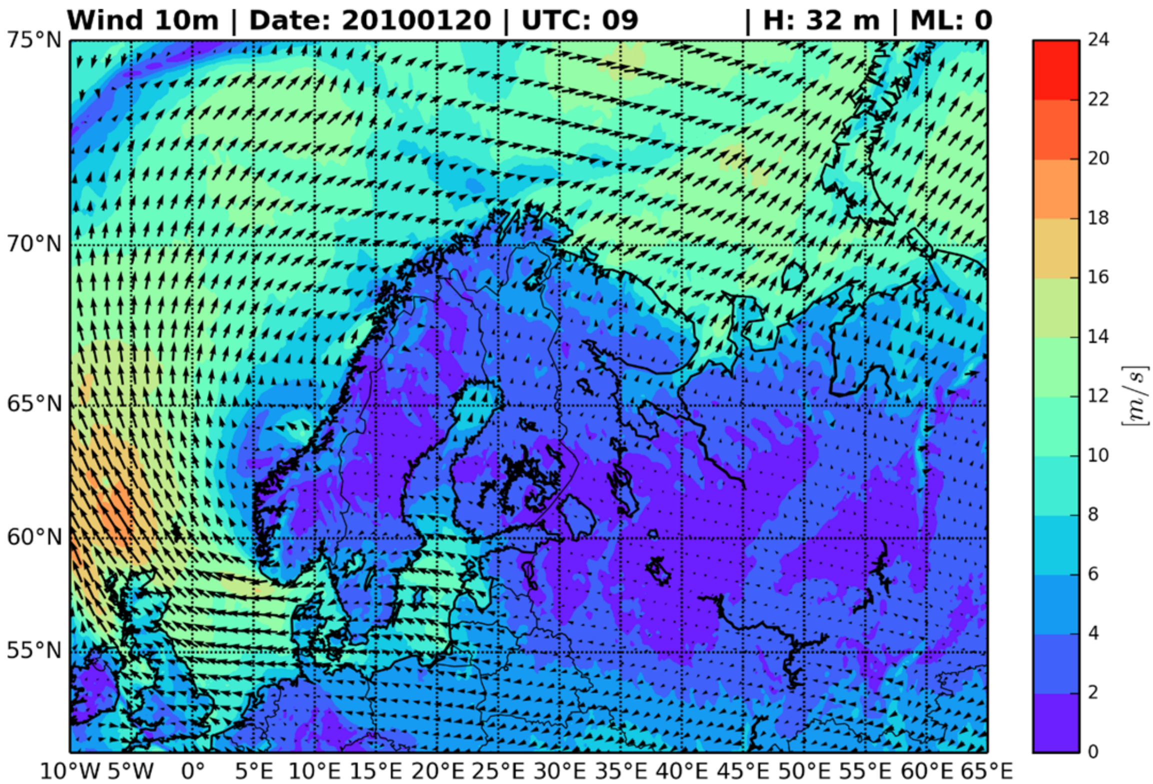


Figure 17. Wind, 10 meters above the ground surface.

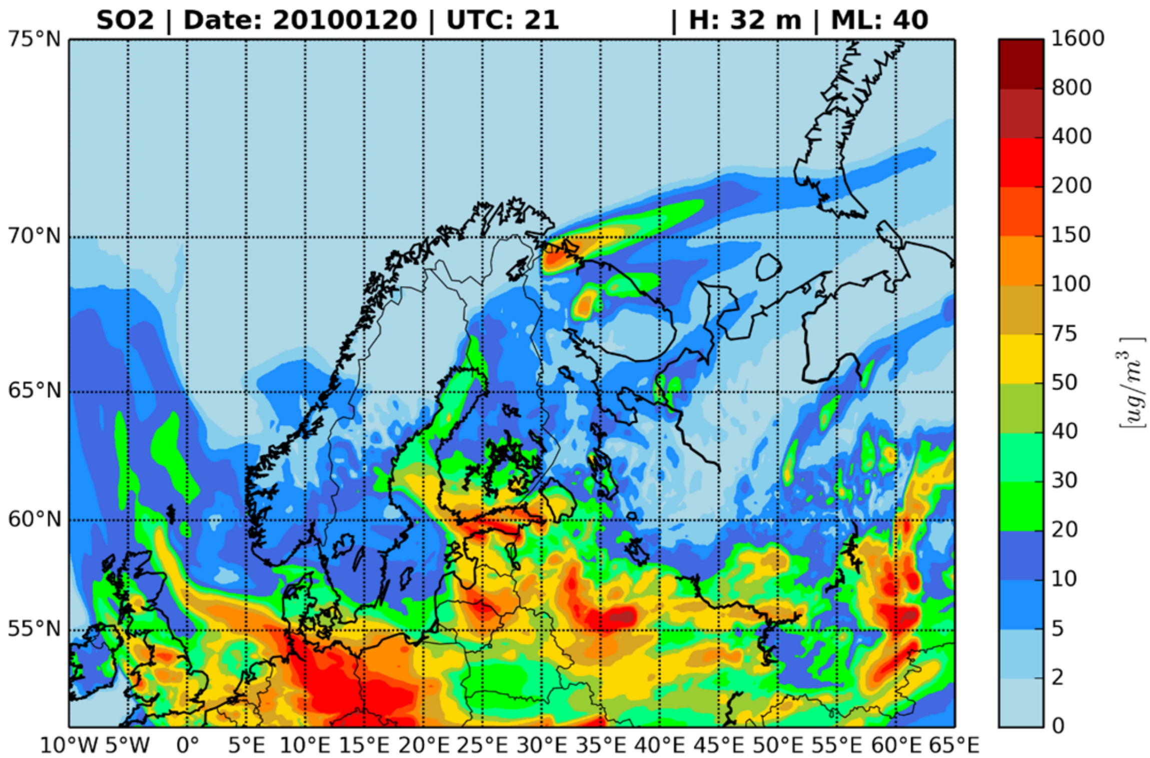


Figure 18. The concentration of sulfur dioxide (SO_2) without adding an additional amount of pollution (e.g. Cu-Ni smelters doubled emissions scenario).

3.2. SO_2 Variability due to Scenarios of Emissions

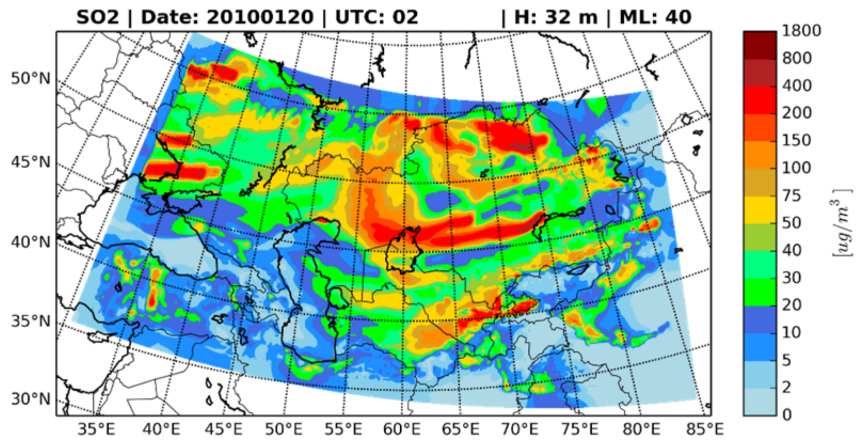
After including addition of source (and amount) of emissions, we conducted a comparative analysis of the results with a control start and showed variability SO_2 concentration for two different scenarios and territories. The first scenario is for an accidental release at the facility near the city of Atyrau (Kazakhstan), and the second scenario is with doubled emissions from usual continuous emissions of SO_2 from three Cu-Ni plants located on the Kola Peninsula.

3.2.1. Accidental release

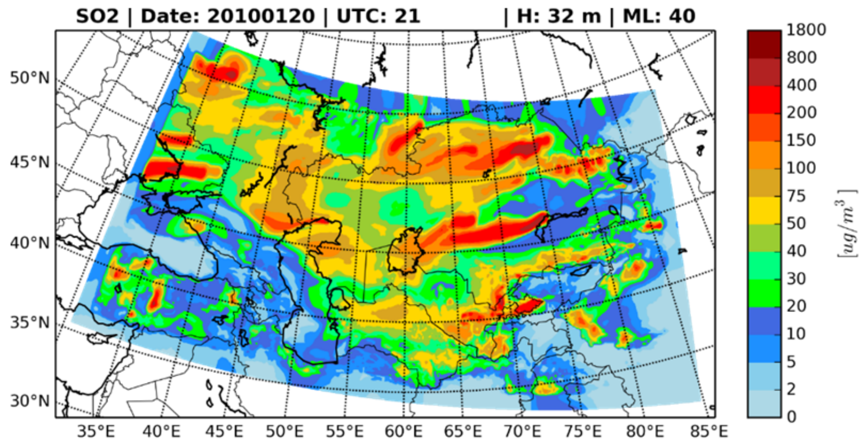
Figures 19 to 20 represent the results of modelling of oil storage reservoir emergency due to fire case that leads to emission of pollutant SO_2 substance into the atmosphere. Figure 19ab shows the modelled SO2 concentration fields at 02 and 21 UTCs on 20th Jan 2010.

As seen in Figure 20, on a diurnal cycle, from the start till the end of the accidental release the pollution cloud was rapidly expanding westward from the source and passing-by over the relatively flat territory northerly of the Caucasus mountains and reaching the Azov Sea area by the end of the first day the release started. The concentration level reached 150 $\mu g/m^3$ in the city of Astrakhan, and in the cities near the Azov Sea level reached 40 $\mu g/m^3$. The concentration cloud was also expanding in northward-southward directions, reaching the territories of Ukraine and the Black Sea, although the concentration levels were lower compared with the main direction of atmospheric transport.

During the entire period studied, he results of simulations during the chosen dates the eastern wind prevailed. So, that, in consequence, the dominated wind transported the pollution from the accident location to the territories of the neighbouring countries.



a)



b)

Figure 19. The concentration of sulfur dioxide (SO_2) in case of emergency in an oil storage at 02 and 21 UTCs on 20th Jan 2010.

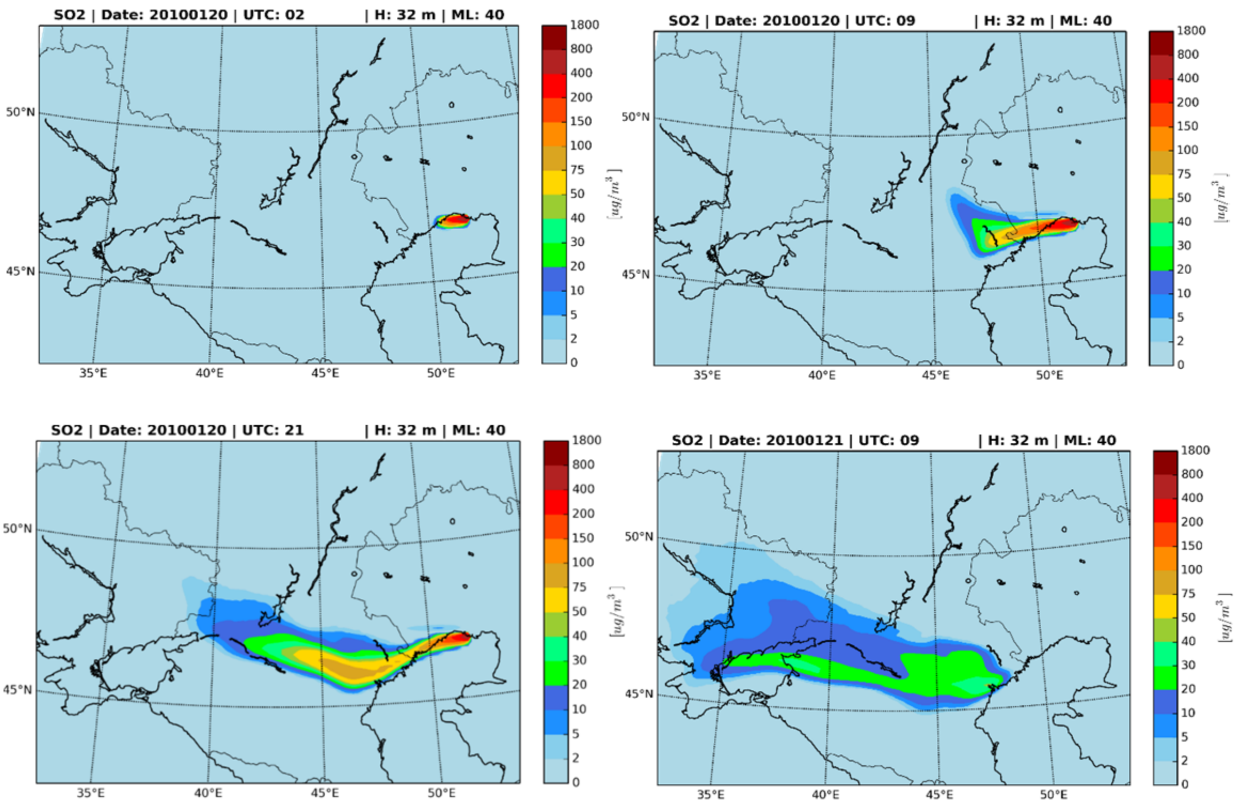


Figure 20. The difference in the concentration of sulfur dioxide (SO_2) between the control and the accidental release (at the Atyrau refinery) runs at the first model level of 32 m above the surface for selected UTC times during 20-21 January 2010.

3.2.2. Continuous emissions

Figure 21 represents the simulation result for Northern Europe at SO_2 emission increase up to 60 thousands tones/year from factories of the Kola MMC. It shows the modelled SO2 concentration fields at 02 and 21 UTCs on 20th Jan 2010.

As seen in Figure 21, from the start till the end of the continuous emissions cloud was rapidly expanding I the north-east from the source, and went towards the Barents Sea reaching the Novaya Zemlya archipelago. The concentration level reached 20 µg/m^3 in the Yuzhny Island. During the entire period studied, he results of simulations during the chosen dates the south-western wind prevailed. So, that, in consequence, the pollution from the continuous emission source does not reach the European countries.

a) b)

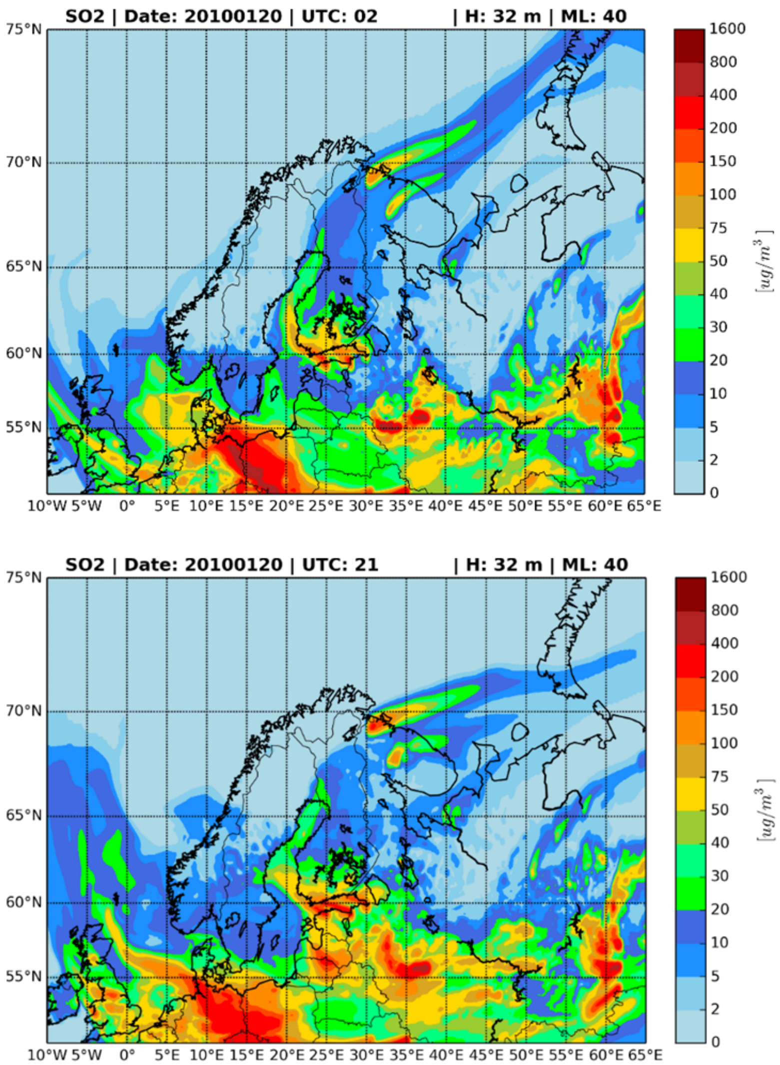


Figure 21. The concentration of sulfur dioxide (SO_2) from continuous sources of pollution at 02 and 21 UTCs on 20th Jan 2010.

Figure 22 represents the concentration difference of SO_2 at emission increase up to 60 thousands tones/year from the current emission amount is obtained from the data base of the GAINS model.

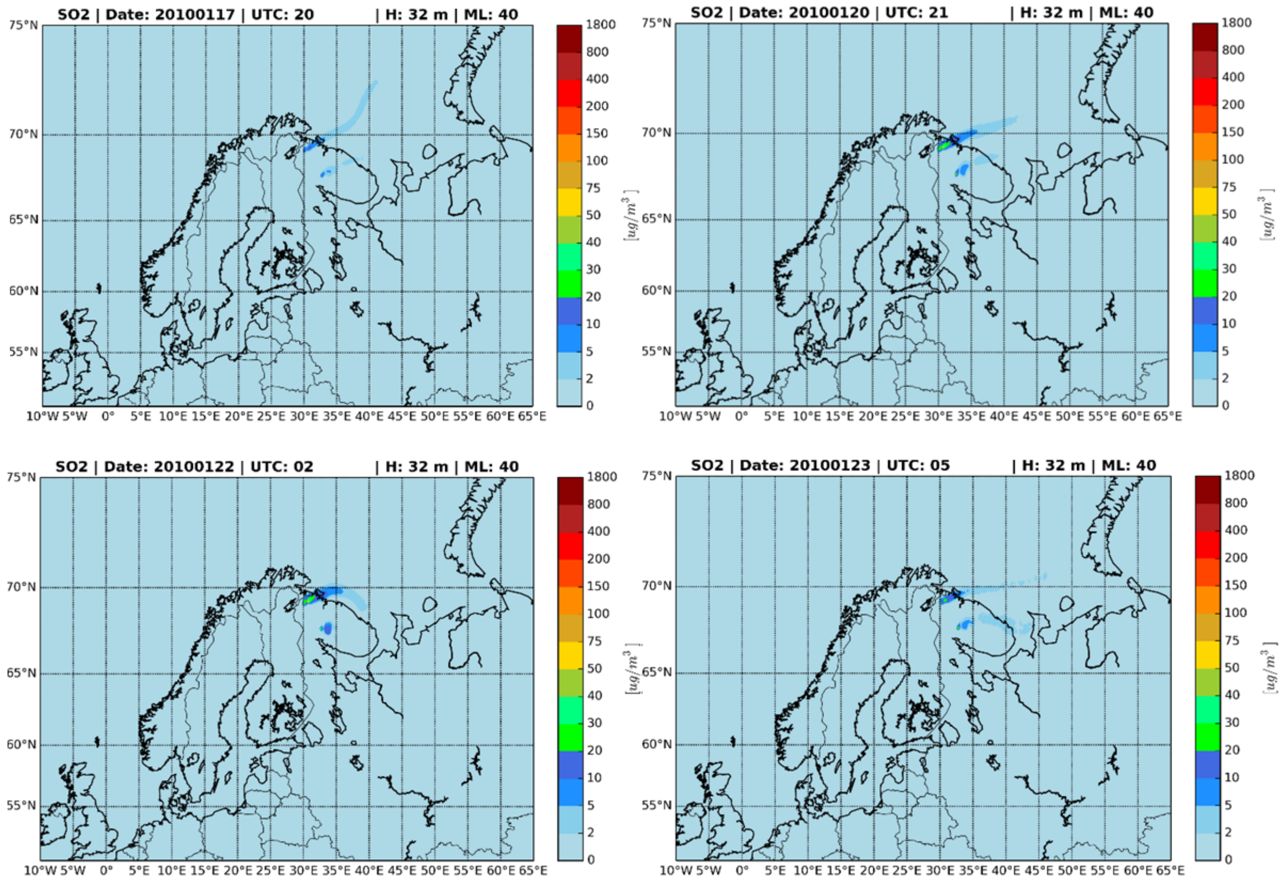


Figure 22. Concentration difference of SO_2 at 60 thou. tonnes/year from current emission.

3.3. Potential Impact on Selected Cities

Using obtained results of modeling, the time series of SO_2 concentration for selected cities of Kazakhstan and European countries were constructed for 30 cities in Kazakhstan and 49 cities in Europe. The MPC (maximum permissible concentration) in the air for the maximum one time dose is 0.5 mg/m³, and the average is 0.05 mg/m³. As we can see from Figure 23, the maximum one time concentration, which is marked as the red dashed line, exceeded 500 µg/m^3 only for a few (7) cities during the studied period. These cities are Balkhash, Ekibastuz, Pavlodar, Shakhtinsk, Saran, Karaganda, and Almaty. The lowest concentrations were obtained for 5 cities – Petropavlovsk, Taldykorgan, Turkestan, Zhanaozen, Kentau, and concentrations did not exceeded there 100 µg/m^3. As seen in time-series, the concentration levels varied substantially during the period studied. Such variability depends on level of emissions from the near-by and/ or remote sources, dominated atmospheric transport pathways from the emission sources and prevailing wind direction characteristic for the cities, possible contribution of removal processes as well as chemical transformations occurred during transport, etc.

Figure 24 represents the daily cycle for the same cities in Kazakhstan. As seen for two cities – Ekibastuz and Balkhash – the indexes are mostly exceed the MPC. For industrialized city of Ekibastuz, the concentration level was always above 400 µg/m^3 on a diurnal cycle. It was lower than 500 µg/m^3 during 04-09 hour and higher than 500 µg/m^3 during the rest of the day. The absolute maximum of 650 µg/m^3 was registered at 19 hour. For Balkhash, the concentration level was always above 290 µg/m^3 on a diurnal cycle. It was lower than 500 µg/m^3 during 02-15 hour and higher than 500 µg/m^3 during the rest of the day. The absolute maximum of 690 µg/m^3 was registered at 22 hour. On a diurnal cycle, the smallest concentrations were seen for 5 cities –

Petropavlovsk, Taldykorgan, Turkestan, Zhanaozen and Kentau among analyzed. It did not reach level of 65 μg/m^3. The largest variability of 400 μg/m^3 was seen for Balkhash among analyzed. It reached a level of 690 μg/m^3. The smallest variability of 4 μg/m^3 was seen for Petropavlovsk among analyzed. It did not reach a level of 13 μg/m^3.

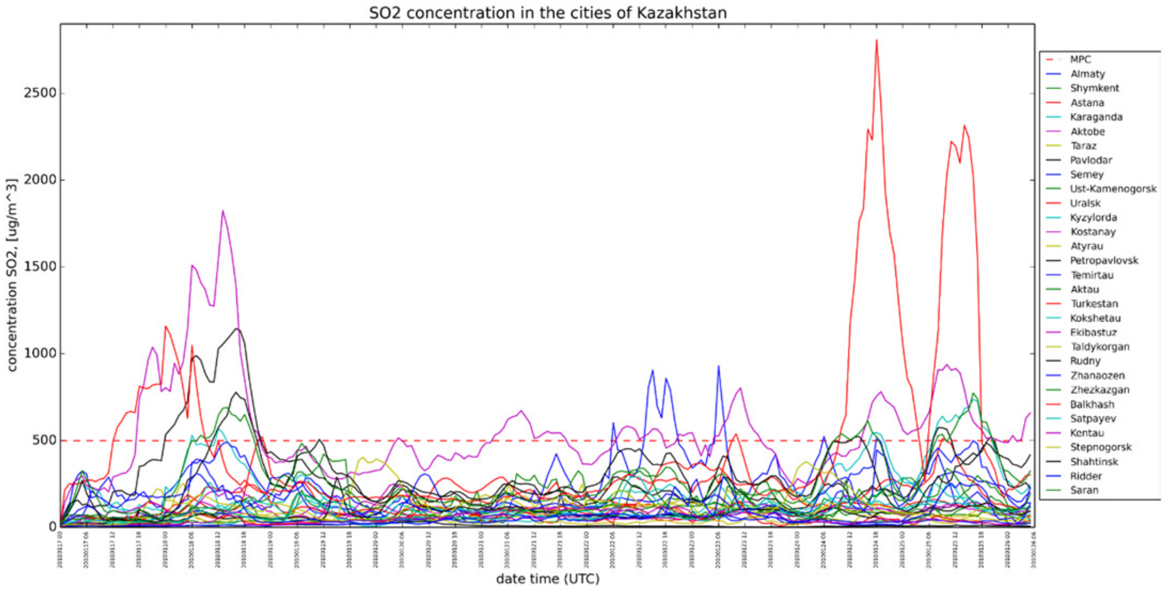


Figure 23. Time series of SO_2 concentration in the cities of Kazakhstan.

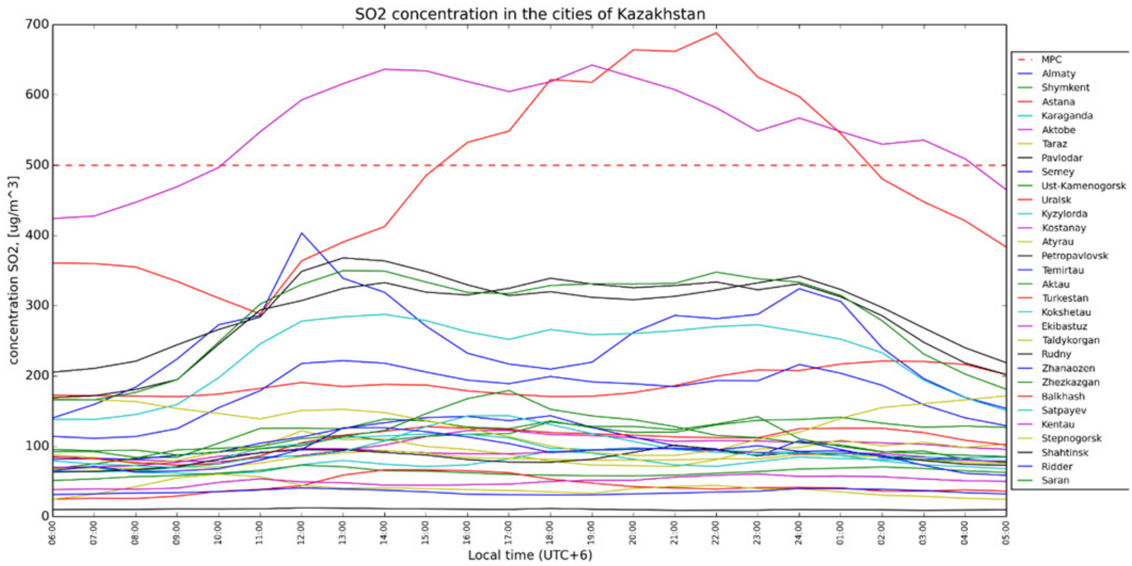


Figure 24. Daily cycle of SO_2 concentration in the cities of Kazakhstan.

The same analysis was done for the cities in Europe, and as we can see from the Figures 25 and 26 the maximum one time concentration, which is marked as the red dashed line, exceeded 500 μg/m3 only two cities during the studied period. The apparent leaders among the most polluted cities are Moscow and Belgrade. The lowest concentrations were obtained for 6 cities – Oslo (Norway), Lisbon (Portugal), Berne (Switzerland), Monaco (Monaco), Andorra la Vella (Andorra), Vaduz (Liechtenstein), and concentrations did not exceeded there 45 μg/m^3.

Figure 26 represents the daily cycle for the same cities in Europe countries. As seen for two cities – Moscow and Belgrade – the indexes are mostly exceed the MPC. For the capital of the Russian Federation Moscow, the concentration level was always above 450 μg/m^3 on a diurnal cycle. It was lower than 500 μg/m^3 during 00-05 hour and higher than 500 μg/m^3 during the rest of the day. The absolute maximum of 820 μg/m^3 was registered at 10 hour. For Belgrade, the concentration level was always above 600 μg/m^3 on a diurnal cycle. It was higher than 500 μg/m^3 during the all day. The absolute maximum of 1250 μg/m^3 was registered at 09 hour. On a diurnal cycle, the smallest concentrations were seen for 3 cities – Lisbon, Andorra la Vella and Vaduz among analyzed. It did not reach level of 12 μg/m^3. The largest variability of 650 μg/m^3 was seen for Belgrade among analyzed. It reached a level of 1250 μg/m^3. The smallest variability of 2 μg/m^3 was seen for Andorra la Vella among analyzed. It did not reach a level of 5 μg/m^3.

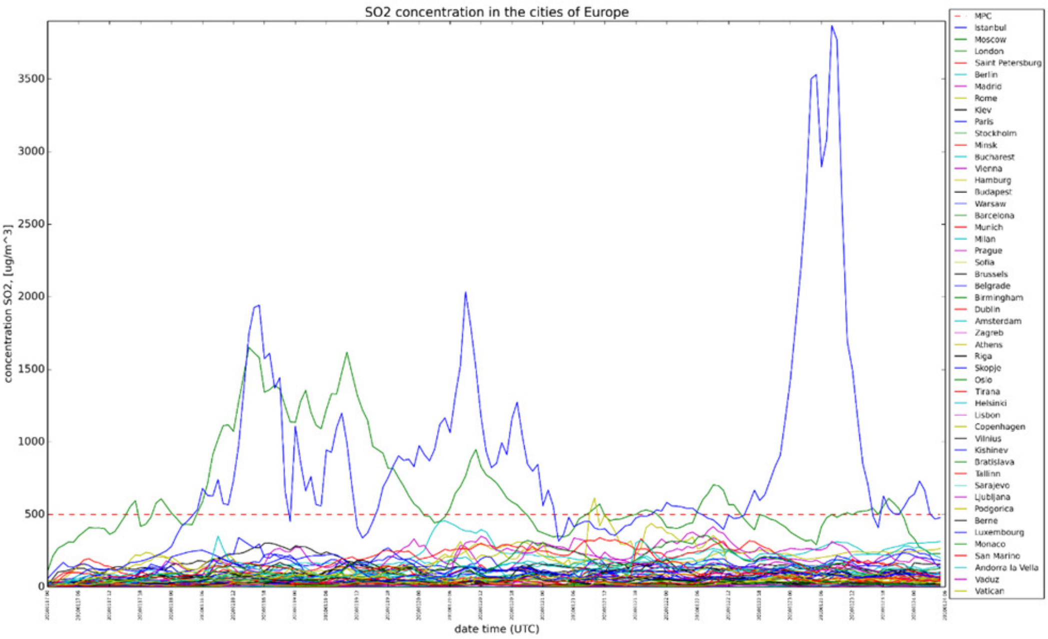


Figure 25. Time series of SO_2 concentration in the cities of Europe.

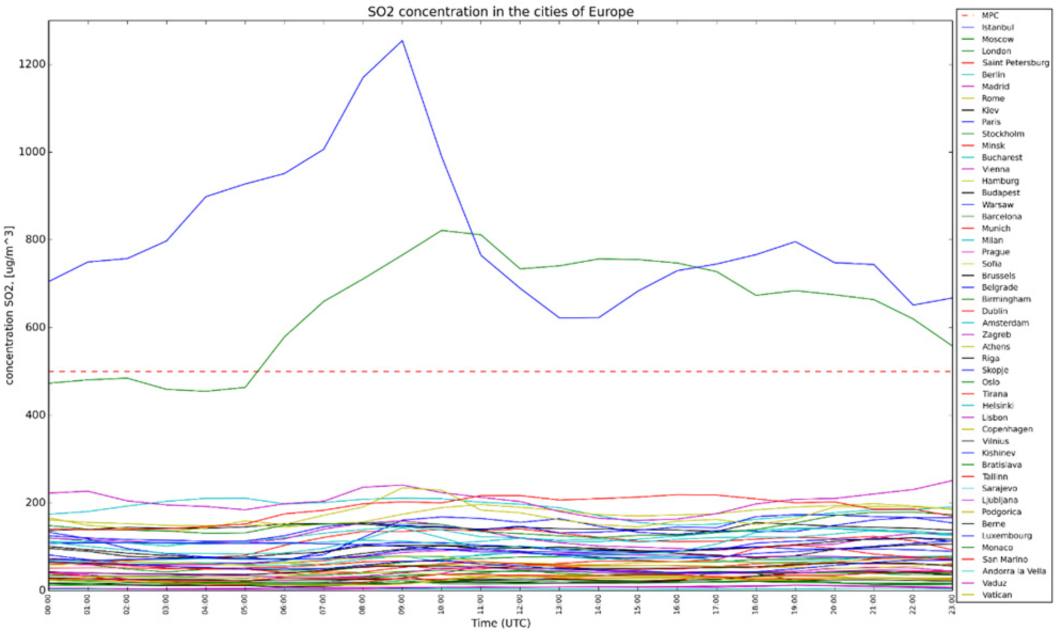


Figure 26. Daily cycle of SO_2 concentration in the cities of Europe.

3.4. Integration and Assessment with GIS Tools

Example of the risk assessment mapping on population is shown in Fig. 27. To construct such map a population density database is combined with averaged accumulated sulfur dioxide concentrations following accidental release (e.g. scenario 1) in Kazakhstan oil refinery employing QGIS, and then the result is integrated into the RANDOM system.

As seen in Figure 27, the area of sulfur dioxide concentrations covered the neighboring countries, in particular, the territory of Russia and Ukraine. This figure shows the whole covered area by the polluting cloud, and the level of its impact on the population. The risk assessment on population map covers the SO_2 concentration field for the period from 00 UTC 20 January 2010 to 23 UTC 22 January 2010. As seen in Figure, a pollution cloud was rapidly expanding westward from the outset of an accidental release until the disappearance covering of the territory from the Caspian Sea in the East to the Black Sea in the West, and from the Caucasus Mountains in the South to the cities Volgograd in Russia and Kiev in Ukraine. The greatest impact, as seen as was caused to the population of cities – Astrakhan, Rostov-on-Don, and Mariupol. The scale has been normalized with relative to maximum value and it was taken as 100%. This value has reached the Rostov-on-Don city. The level more than 50% are also included the cities as Astrakhan, Mariupol, Donetsk, and Sevastopol. The rest of the cities is below the level of 50%.

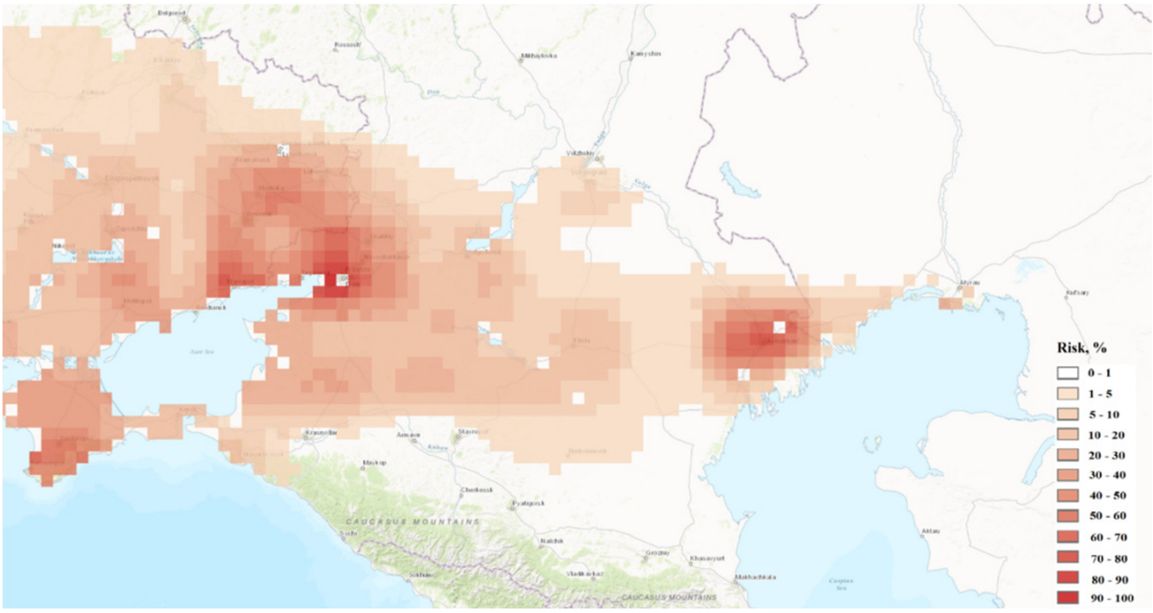


Figure 27: Population risk mapping integrated into RANDOM system.

4. Conclusions

In this study, investigation of different scenarios (accidental discharges and continuous emissions) was performed by analysis of atmospheric transport, dispersion and sedimentation of contaminants using an online integrated model of meteorology, chemistry/aerosols of Enviro-HIRLAM adapted and configured for the two areas of interest: Kazakhstan and Europe.

Calculations were made on different scenarios of short-term modeling of meteorology and chemical fields used for comparative analyzes, calculations with respect to accidental pollution of the atmosphere and to continuous emissions from copper-nickel factories. In addition, calculations with the same parameters, but with a finer horizontal resolution (Downscaling) for the territory of the Caspian Sea. The result obtained by spatio-temporal fields of SO_2 concentration, with a time step of 1 hour for the calculation period from 17 till 26 Jan 2010. The data were visualized allowing to construct distribution maps and pollution levels in the study area. In case of an accidental release from the Atyrau refinery, the pollution cloud reached the Azov Sea in the west of the source. For continuous emissions modeling from the Kola Peninsula sources, the cloud reached the territories of the Novaya Zemlya archipelago.

The concentration of sulfur dioxide field was analyzed and the level of the pollutant was assessed for the cities of Kazakhstan and Europe. The most polluted cities of the two regions have been identified from the evaluation of time series of modeled concentrations of sulfur dioxide and precipitation in major populated cities, some regions and countries. For Kazakhstan, the most polluted cities identified were Balkhash and Ekibastuz, and the least - Petropavlovsk and Taldykorgan. The clear leaders among the European polluted cities are Moscow and Belgrade, and with the lowest concentration of sulfur dioxide of Andorra la Vella and Vaduz.

Employing the GIS tools, the risk maps of the impact of sulfur dioxide to the urban population of Kazakhstan and neighboring countries were composed. Pollution cloud expanded over territories of Russia and Ukraine, reaching the Azov Sea aquatoria, and the impact was seen on cities such as Astrakhan, Rostov-on-Don, Mariupol, Donetsk, and Sevastopol.

The model calculates the set of meteorological and chemical parameters that allows for the analysis of other meteorological parameters and pollutants that have not been reflected in this study. The model was used for the first time in Kazakhstan, and there are plans to continue use this model for the Kazakhstan domain in other research applications.

Acknowledgements

This pilot study has been performed during the research PhD training at the Research and Development Department of the Danish Meteorological Institute (RDD DMI, Copenhagen, Denmark) in Nov-Dec 2015. The DMI HPC CRAY-XT5 supercomputing facilities have been used extensively in this study as well as ECMWF meteorological data archives. The project was conducted in collaboration with the DMI and University of Copenhagen. I would like to gratefully thank the DMI for providing the office space and supercomputer to work on research and modelling as integral part of the PhD thesis. It has been rewarding to be a part of the research environment at the DMI.

I would like to express my gratitude to my supervisors - Prof. Alexander Baklanov, Drs. Alexander Mahura and Roman Neuterman - for inspiration and guidance through this study realized. Thanks to colleagues of the DMI's RDD for useful discussions, and IT DMI Department for technical support and advice. This research training was supported through the funding provided by the KazNRTU and IITU (Almaty, Kazakhstan).

References

Baklanov, A., 2008. Integrated Meteorological and Atmospheric Chemical Transport Modeling: Perspectives and Strategy for HIRLAM/HARMONIE. HIRLAM Newsletter, 53.

Korsholm, U.S., Baklanov, A., Gross, A., Mahura, A., Sass, B.H., Kaas, E., 2008. Online coupled chemical weather forecasting based on HIRLAM – overview and prospective of Enviro-HIRLAM. HIRLAM Newsletter, 54.

Mahura, A., Sattler, K., Petersen, C., Amstrup, B., Baklanov, A., 2006. DMI-HIRLAM Modelling with High Resolution Setup and Simulations for Areas of Denmark. Technical Report 05-12.

Mahura, A., Gonzalez-Aparicio, I., Nuterman, R., Baklanov, A., 2012. Modelling and Evaluation of Impact on Population due to Continuous Emissions from the Severonickel Smelters (Kola Peninsula). Research Paper, Copenhagen, Denmark.

Zakarin, E., Balakay, L., Mirkarimova, B., Mahura, A., Baklanov, A., Sorensen, J., 2012. Transboundary Atmospheric Pollution of Oil-Gas Industry Emissions from North Caspian region of Kazakhstan. Abstract EGU-2012.

Zakarin, E., Balakay, L., Dedova, T., Kim, D., 2015. Development of risk mapping system for flora and fauna in the north Caspian Sea. Science, Technology, Industry, VI (10)

Nuterman, R., Korsholm, U., Zakey, A., Nielsen, K., Sorensen, B., Mahura, A., Rasmussen, A., Mažeikis, A., Gonzalez‐Aparicio, I., Morozova, E., Sass, B.H., Kaas, E., Baklanov, A., 2013. New Developments in Enviro‐HIRLAM online integrated modeling system. Geophysical Research Abstracts, 15, EGU2013‐12520.

Baklanov, A., Mahura, A., Sokhi, R. (eds.), 2010. Integrated Systems of Meso-Meteorological and Chemical Transport Models. Springer, 192p.

RANDOM system - http://ecorisk.kz