Multiscale numerical simulation of pollution transport in near surface air

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NWP & AQ simulation

Nowadays a broad range of problems of atmospheric physics, climate and environment protection is solved with application of mathematical modelling approach. Modelling systems, developed at large centres of atmospheric research, are applied for scenario analysis, weather prediction, air quality investigation.

For example,

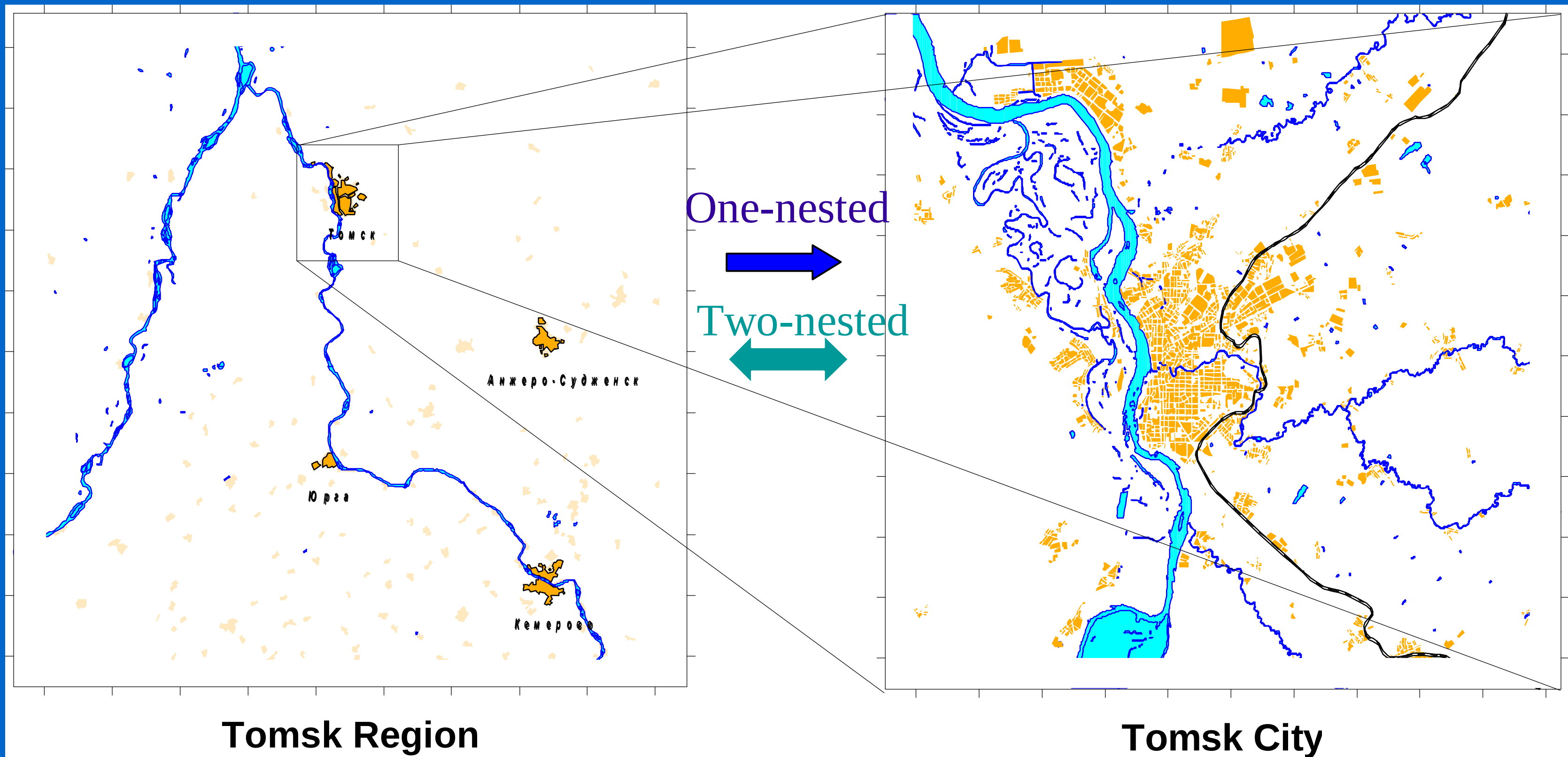
CMAQ, Community Multiscale Air Quality Chemical Transport Modelling System;

EURAD, EURopean Acid Deposition model,

EZM, European Zooming Model.

Dynamic core of such systems are or well-known models (e.g. MM5, WRF) either original models.

Nesting technology



Domain 200x200km^2

Domain 50x50 km^2

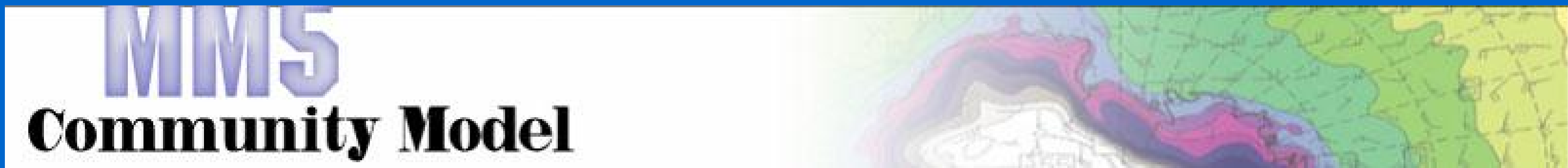
MM5 (Mesoscale Model 5)

The PSU/NCAR mesoscale model is a limited-area, nonhydrostatic or hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale and regional-scale atmospheric circulation. It has been developed at Penn State and NCAR as a community mesoscale model.

The Fifth-Generation NCAR / Penn State Mesoscale Model (MM5) includes a multiple-nest capability, nonhydrostatic dynamics, which allows the model to be used at a few-kilometer scale, multitasking capability on shared- and distributed-memory machines, a four-dimensional data-assimilation capability, more physics options.

Mesoscale Model 5

MM5 generates meteorological fields:
- horizontal and vertical wind components,
- pressure,
- temperature,
- air humidity,
- cloudiness and precipitation parameters,
- heat, moisture and momentum fluxes,
- short-wave and long-wave radiation.



THE WEATHER RESEARCH & FORECASTING MODEL

The Weather Research and Forecast Model is a next-generation mesocale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs.
It features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility.
The WRF model is a fully compressible, nonhydrostatic model.
Its vertical coordinate is a terrain-following hydrostatic pressure coordinate.
Model uses the Runge-Kutta 2nd and 3rd order time integration schemes, and 2nd to 6th order advection schemes in both horizontal and vertical directions. The dynamics conserves scalar variables.

WRF THE WEATHER RESEARCH & FORECASTING MODEL

The WRF model is designed to be a flexible, state-of-the-art atmospheric simulation system that is portable and efficient on available parallel computing platforms. WRF is suitable for use in a broad range of applications across scales ranging from meters to thousands of kilometres, including:

- Idealized simulations (e.g. LES, convection, baroclinic waves)
- Parameterization research
- Data assimilation research
- Forecast research
- Real-time NWP
- Coupled-model applications
- Teaching

MM5 & WRF

Since the MM5&WRF modeling system are primarily designed for real-data studies/simulations, it requires the following datasets to run:

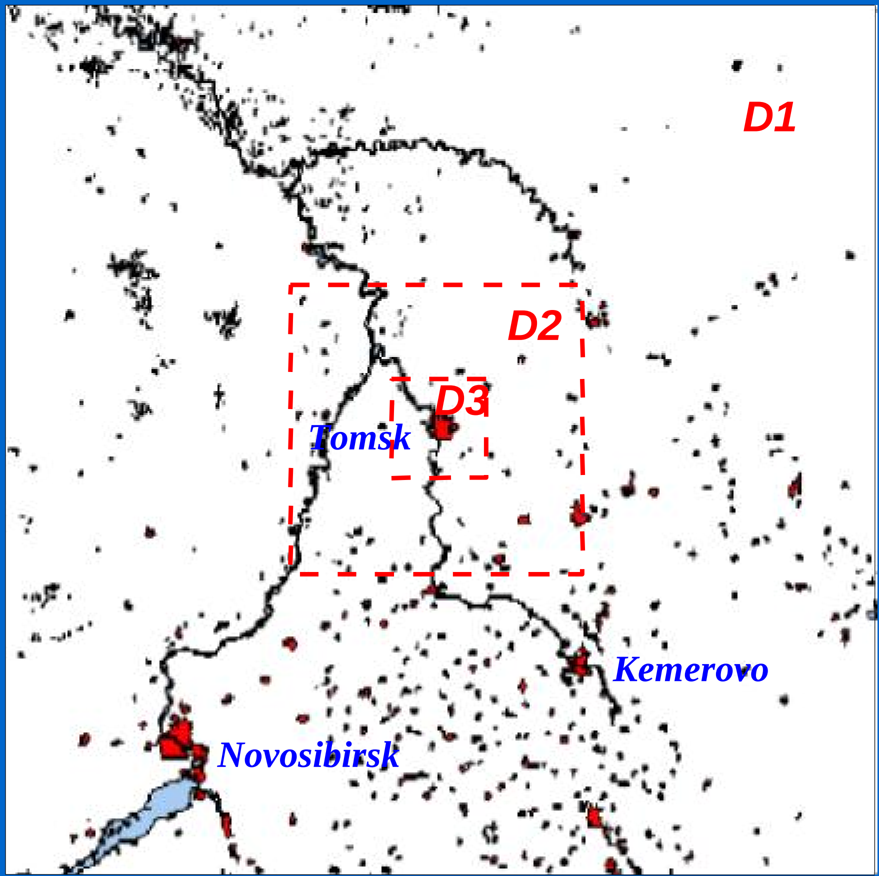
- Topography, landuse and vegetation (in categories);
(1º - 30’’ resolution)
- Gridded atmospheric data that have at least these variables: sea-level pressure, wind, temperature, relative humidity and geopotential height; and at these pressure levels:
surface, 1000, 850, 700, 500, 400, 300, 250, 200, 150, 100 mb;
- Observation data that contains soundings and surface reports (final analysis data NCEP or ECMWF, global data NCEP)

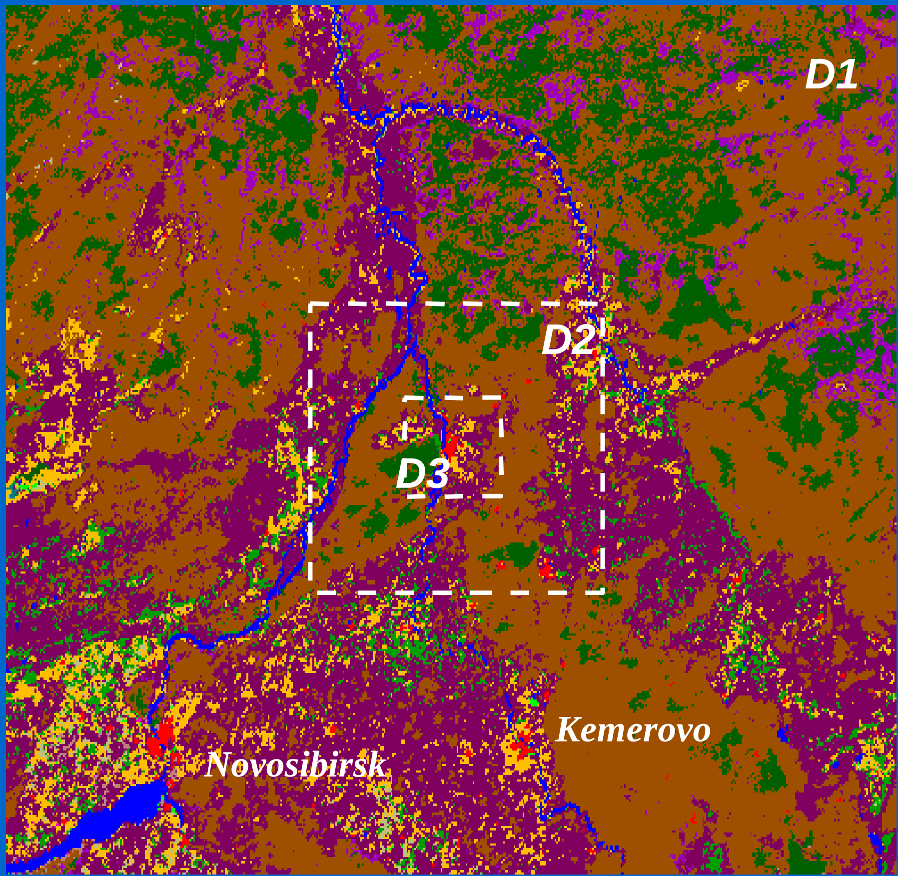
Simulation cases

Two temporal periods: 16-17 May 2004;
20-21 October 2004;
Three local nested domains with horizontal sizes 450x450, 150x150 и 50x50km^2.
South of Western Siberia, Tomsk (56,5^o N, 85^o E) is in the centre of domains;
Initial state of atmosphere and lateral boundary conditions were set up on the basis of NCEP final analysis data


Tomsk (56,6N; 85,0E)
ARCTIC OCEAN
Barents Sea
Kara Sea
Laptev Sea
East Siberian Sea
Bering Sea
Sea of Okhotsk
NORTH PACIFIC OCEAN
Black Sea
Caspian Sea
Aral Sea
Lake Baikal
SIBERIA
URAL MTS.
Arctic Circle
MOSCOW
Saint Petersburg
Kaliningrad
Vyborg
Murmansk
Petrozavodsk
Arkhangel'sk
Nizhniy Novgorod
Kazan'
Rostov
Novorossiysk
Volgograd
Tuapse
Sochi
Astrakhan'
Yekaterinburg
Chelyabinsk
Omsk
Novosibirsk
Krasnoyarsk
Irkutsk
Noril'sk
Yakutsk
Magadan
Anadyr'
Provideniya
Petropavlovsk-Kamchatskiy
Khabarovsk
Kholmsk
Nevel'sk
Nakhodka
Vostochnyy
Vladivostok
KURIL ISLANDS
KAZAKHSTAN
CHINA
MONG.
JAPAN
N. KOR.
UKRAINE
BELARUS
POLAND
GER.
NOR.
SWE.
FIN.
IRAN
0 300 600 km
0 300 600 mi

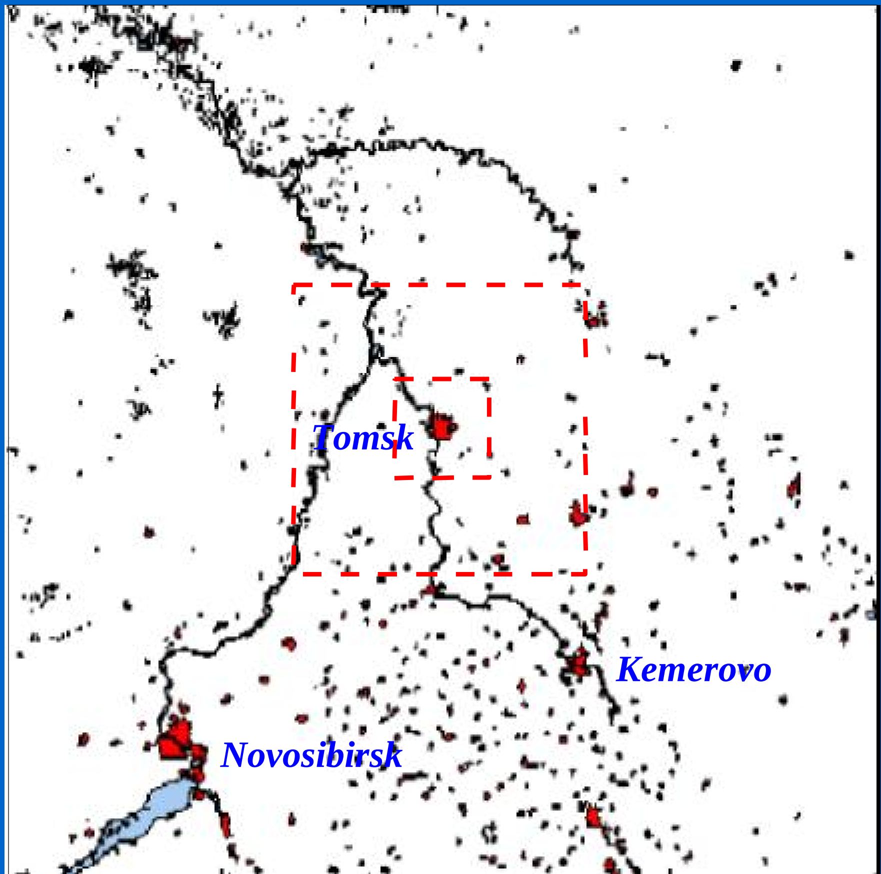
Simulation conditions

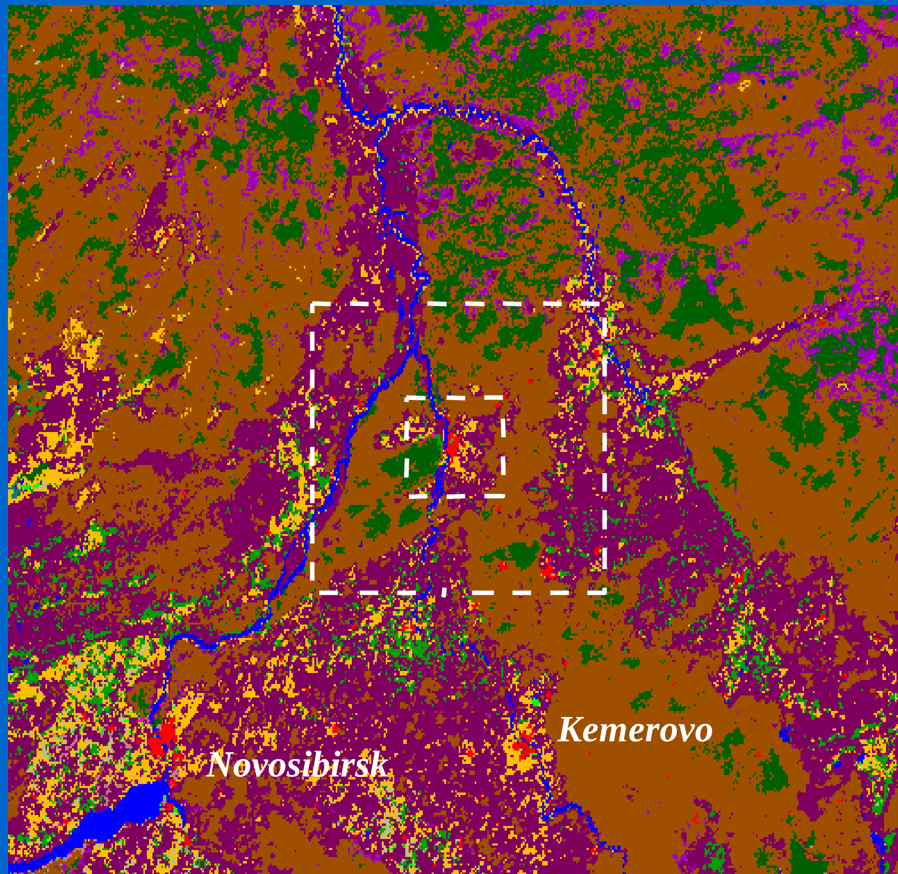




Three nested domains D1, D2, D3 and distribution of landuse categories

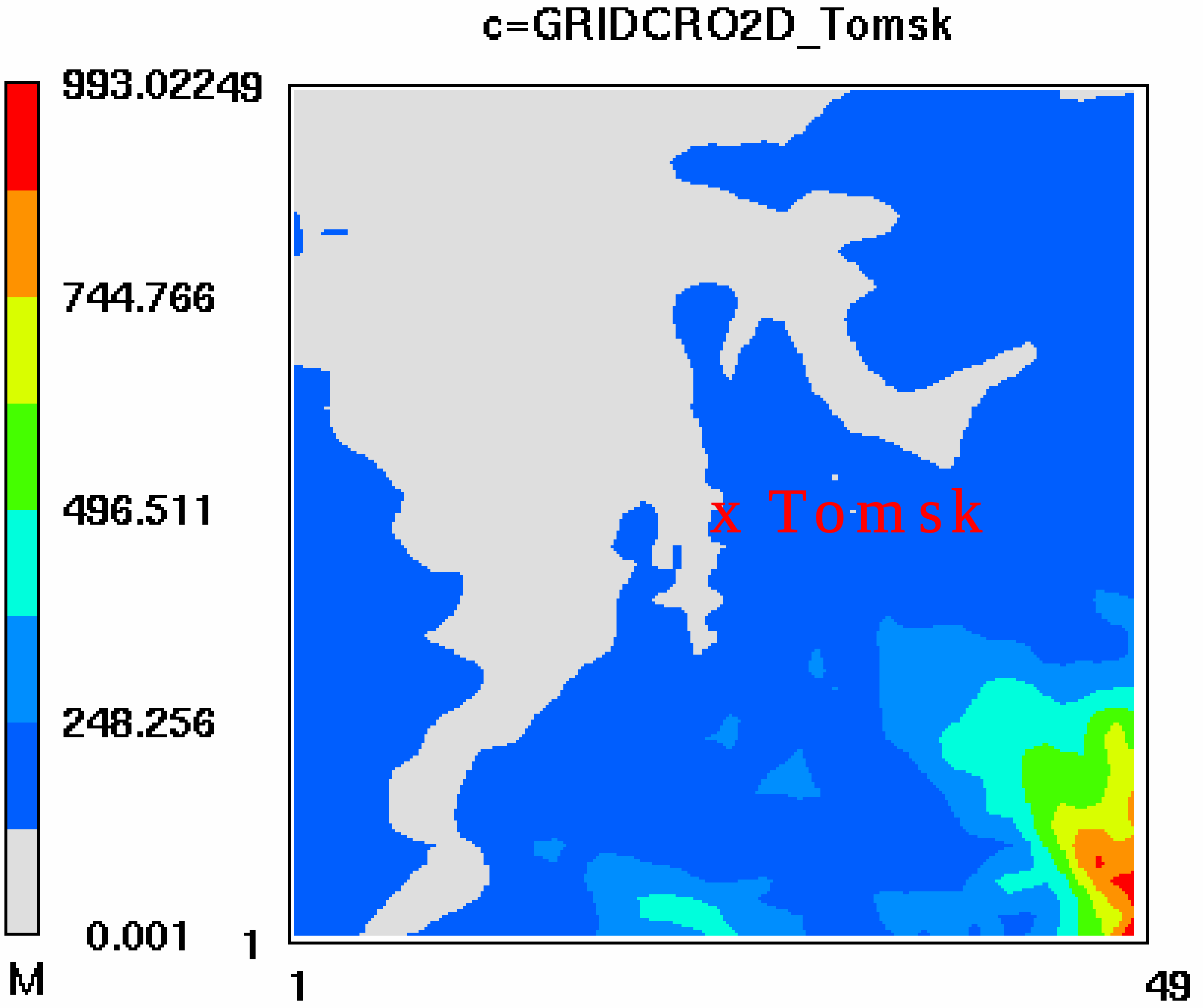
Geographic map and land use distribution





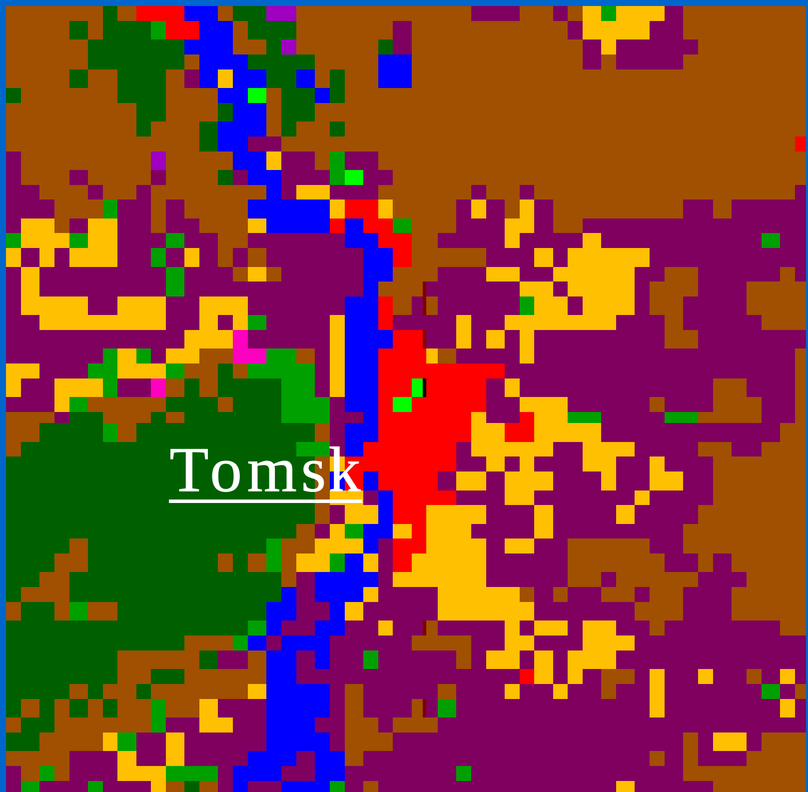
Color table of land use categories in domain 450x450km:
blue-water, violet-few vegetation, yellow-farmland, light green-deciduous forest, brown-mixed forest, green-evergreen forest, red-urban area

Terrain elevation map



450km
x
450km

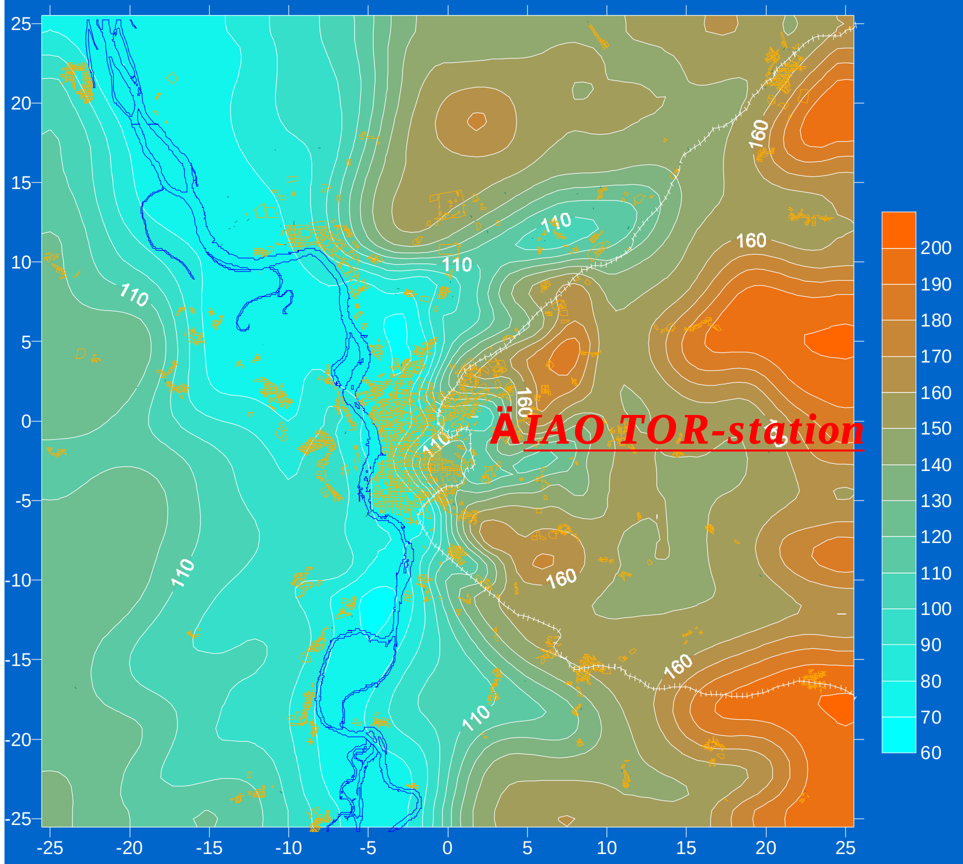
Land use categories for the research domain

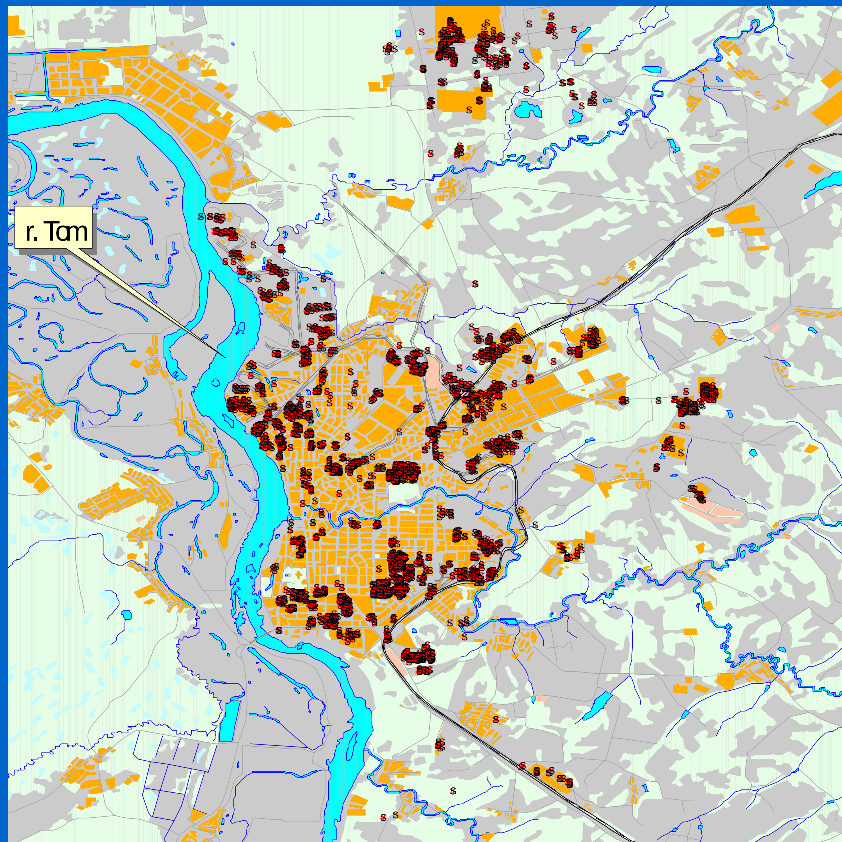


Water
Few vegetation
Farmland
Deciduous forest
Mixed forest
Evergreen forest
Urban area

Tomsk city 50x50 km^2

Surface elevation above sea level and pollution emission distribution in Tomsk





Simulation options

MM5

Grids 52x52x31 for domains D1, D2, D3
Horizontal resolution: 9; 3; 1 km for D1, D2, D3
Temporal step: 27; 9; 3 sec for D1, D2, D3
Vertical size of domains: 17km
Cluster IAO SB RAS

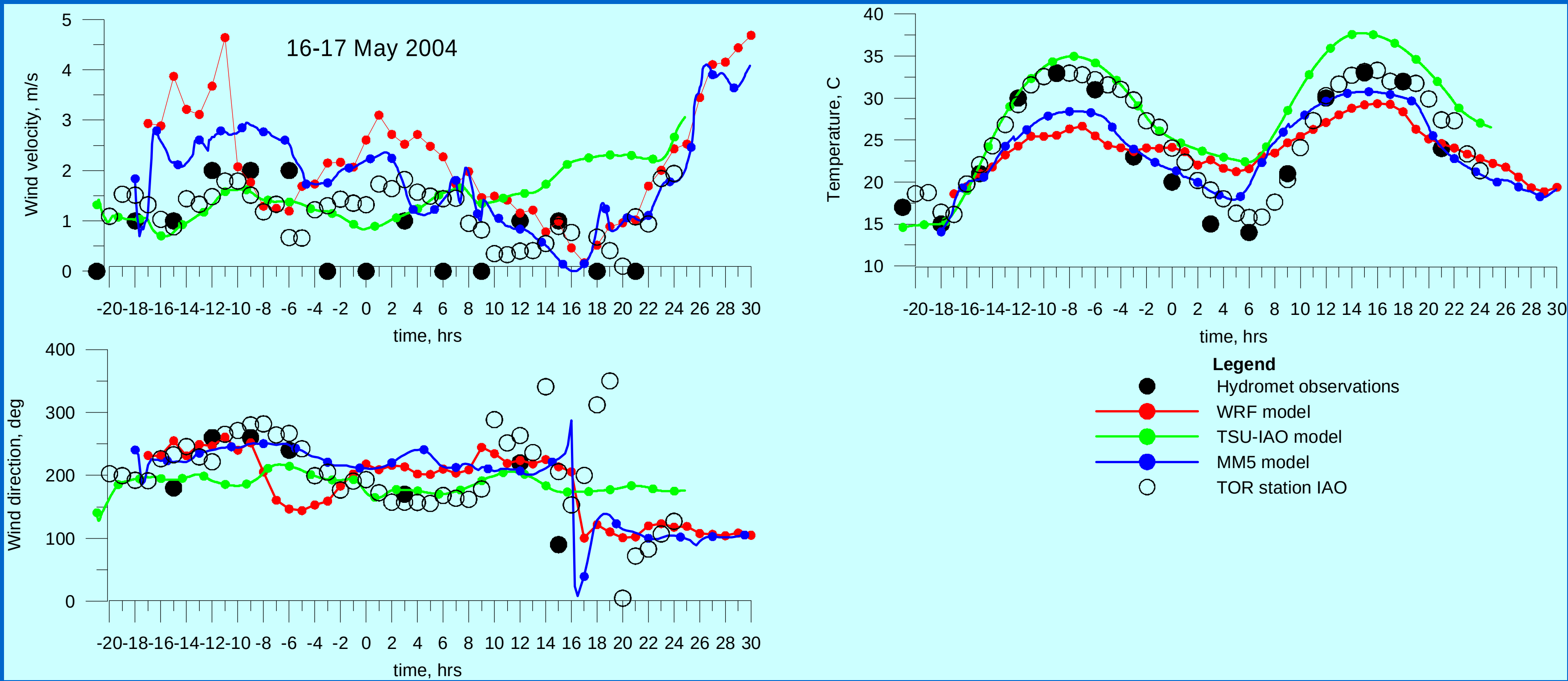
WRF

Grids 52x52x31 for domains D1, D2, D3
Horizontal resolution: 9; 3; 1 km for D1, D2, D3
Temporal step: 60; 30; 10 sec for D1, D2, D3
Vertical size of domains: 17 km
Cluster IAO SB RAS

Simulation options

MM5	WRF
Mixed phase microphysics by Reisner RRTM scheme for long wave radiation Similarity theory for surface layer Thermal diffusion for soil Blackadar scheme for PBL None cumulus parameterization	Eta Grid-Scale Cloud and Precipitation scheme by Ferrier RRTM scheme for long wave radiation Dudhia scheme for short wave radiation Similarity theory for surface layer Thermal diffusion for soil MYJ scheme for PBL

Comparison of the models

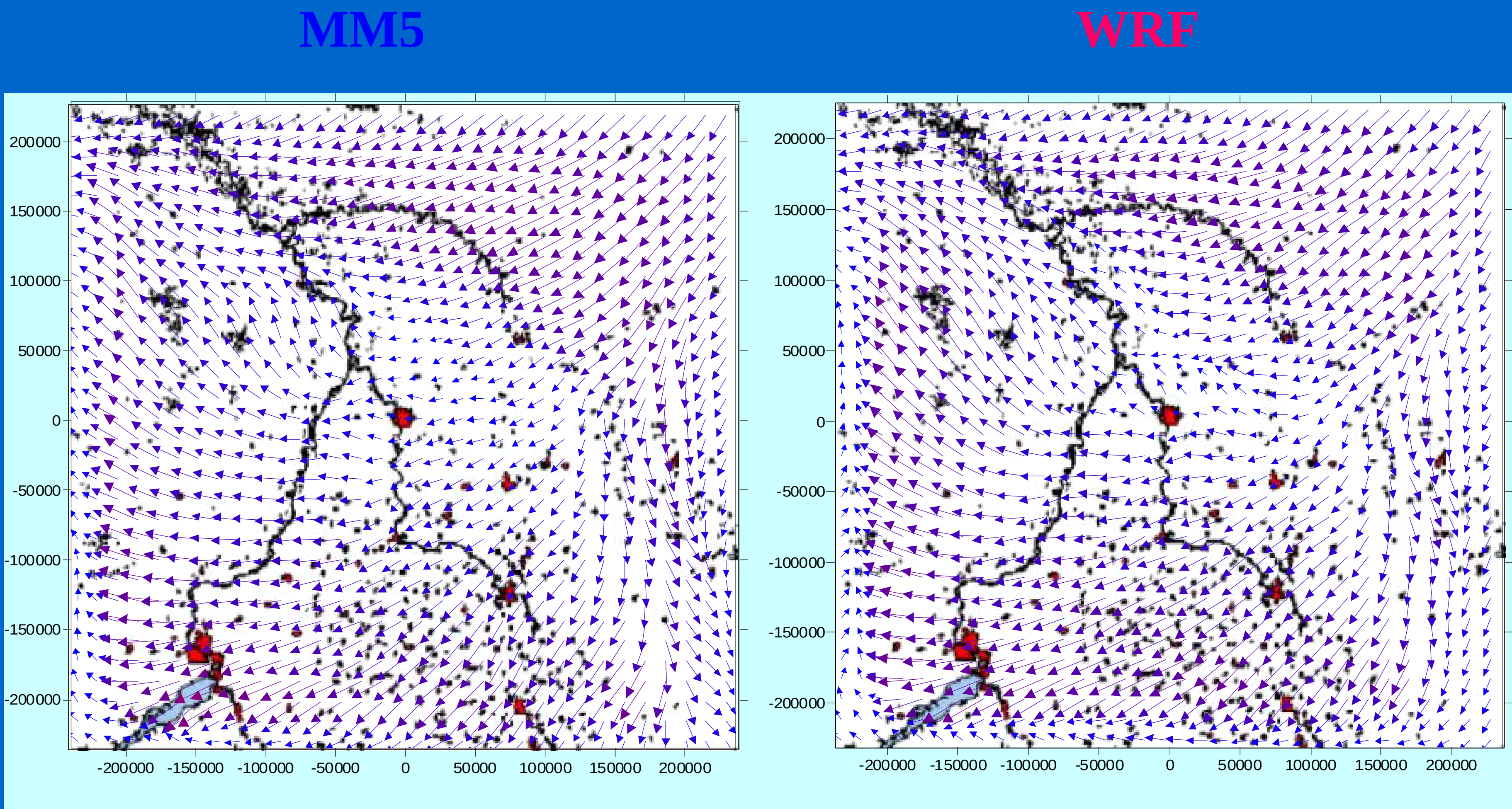


Time=-20…0: 16 May 2004;
Time= 0…24: 17 May 2004

MM5
WRF

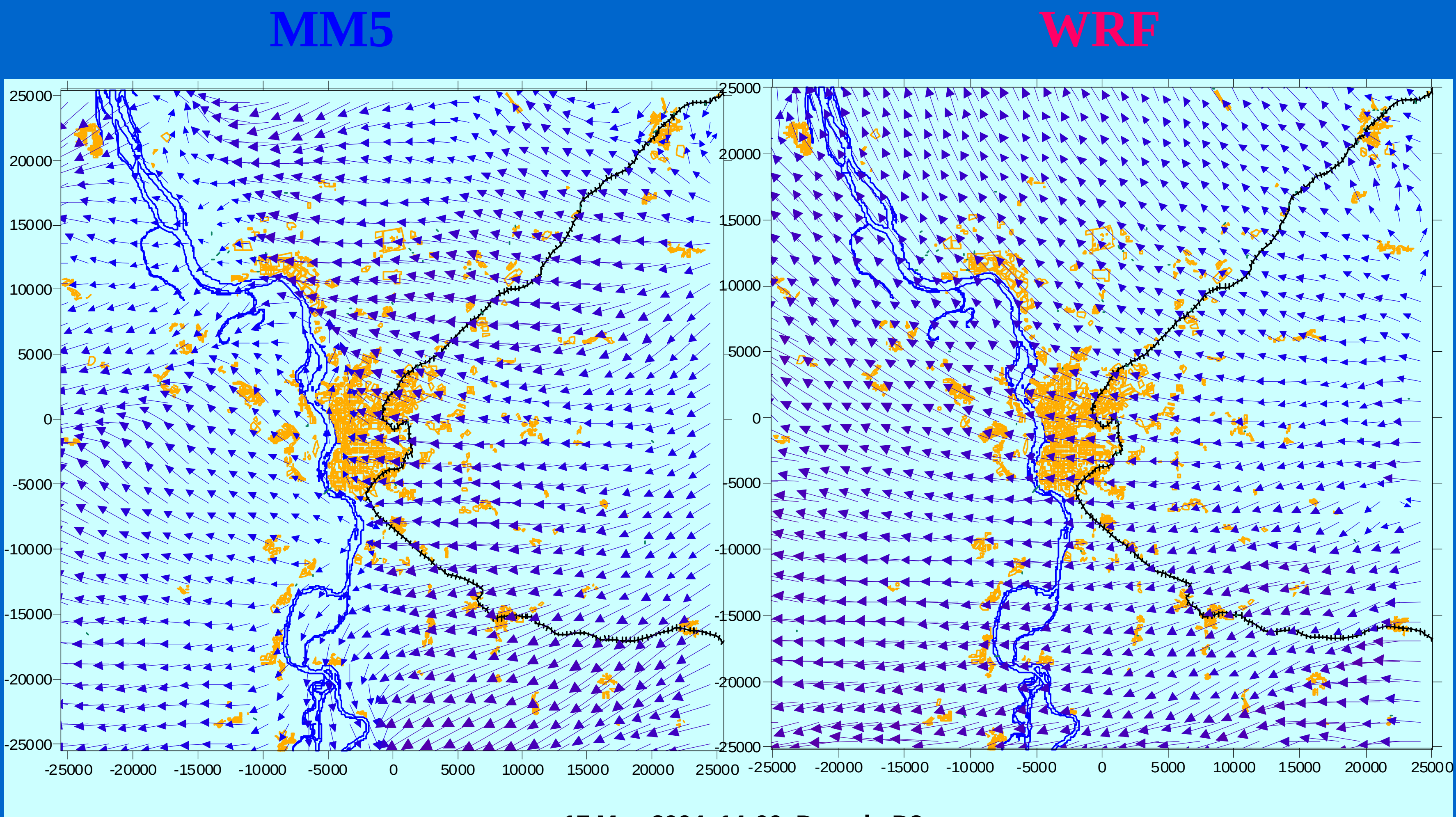
Wind velocity and direction at 10m
Air temperature at 2m in Tomsk

Wind at 10m for the domain D1



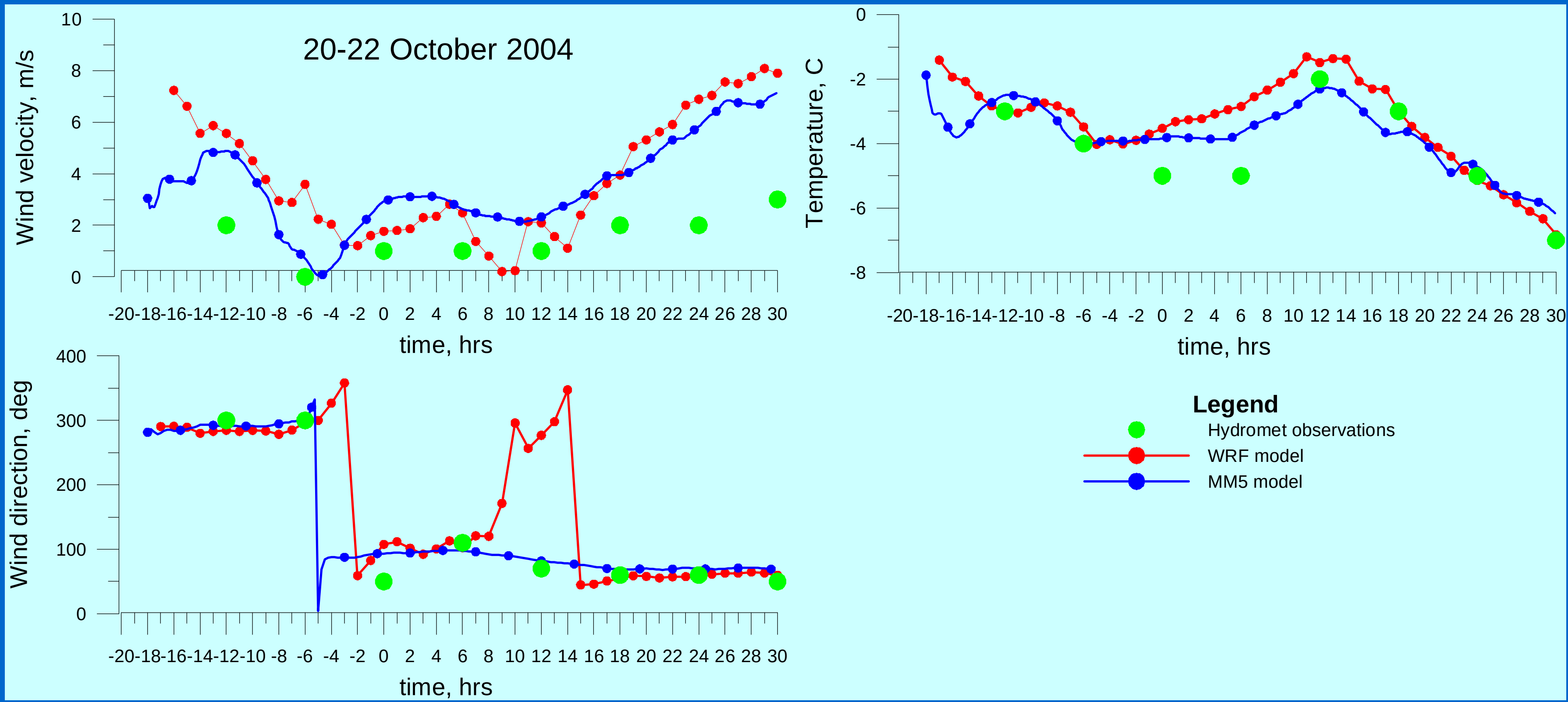
17 May 2004, 14:00, domain 1

Wind at 10m for the domain D3



17 May 2004, 14:00, Domain D3

Comparison of the models

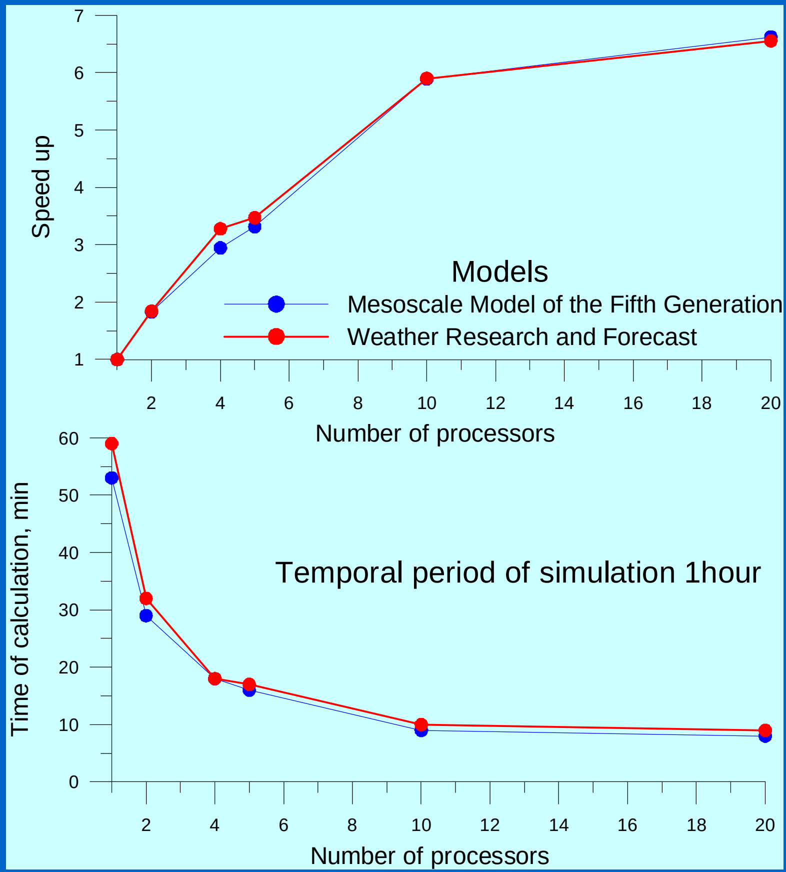


Time=-20…0: 20 October 2004; **MM5**
Time= 0…24: 21 October 2004 **WRF**

Wind velocity and direction at 10m
Air temperature at 2m in Tomsk

Parallel realization of the models

Linux cluster IAO:
10 nodes, each with 2 processors Pentium III 1GHz and RAM 1Gb
Communication net 1Gbs Ethernet, “star” topology
11Gflops on the LINPACK test



MM5 80Mb, WRF 210Mb

CAMx

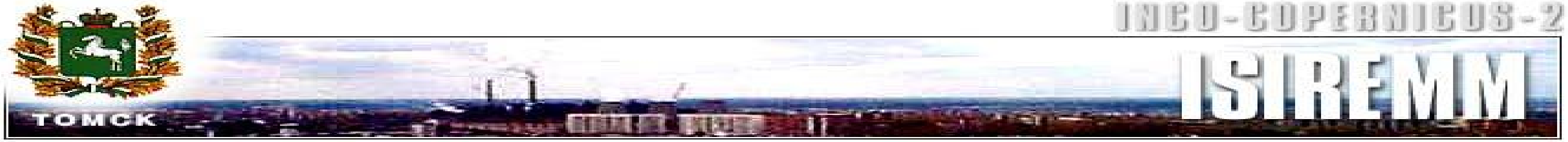
The Comprehensive Air quality Model with extensions (CAMx) is an Eulerian photochemical dispersion model that allows for an integrated “one-atmosphere” assessmen of gaseous and particulate air pollution (ozone, PM2.5, PM10, air toxic, mercury) over many scales ranging from sub-urban to continental.

CAMx simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids.

Four versions of the Carbon Bond IV (CB-IV) chemical mechanis

SAPRC99 mechanism

A computer modeling system TSU-IAO was created within the project *Integrated System for Intelligent Regional Environmental Monitoring & Management in a city/region (on the example of Tomsk region)* of the European Community Framework 5 Program to assist in the analysis of the distribution of meteorological parameters and the concentration of admixtures in the atmospheric boundary layer above a rough inhomogeneous underlying surface. The nonhydrostatic prognostic mesoscale model and the model of pollution transformation and transport make the core of this system.



Components of the MS TSU-IAO

Model initialization block (terrestrial data, ground-based observations, data of vertical distributions of meteorological parameters, data base of point, area and mobile sources of air pollution)

Nonhydrostatic meteorological model

Pollution transport photochemical model

Data visualization block

Model initialization block

Terrestrial data: topography, land use categories (albedo, soil thermal conductivity, heat capacity, density, evaporation, surface roughness, emissivity, deep soil temperature)

Ground-based and vertical observations of wind velocity and wind direction, air temperature and humidity, atmospheric pressure

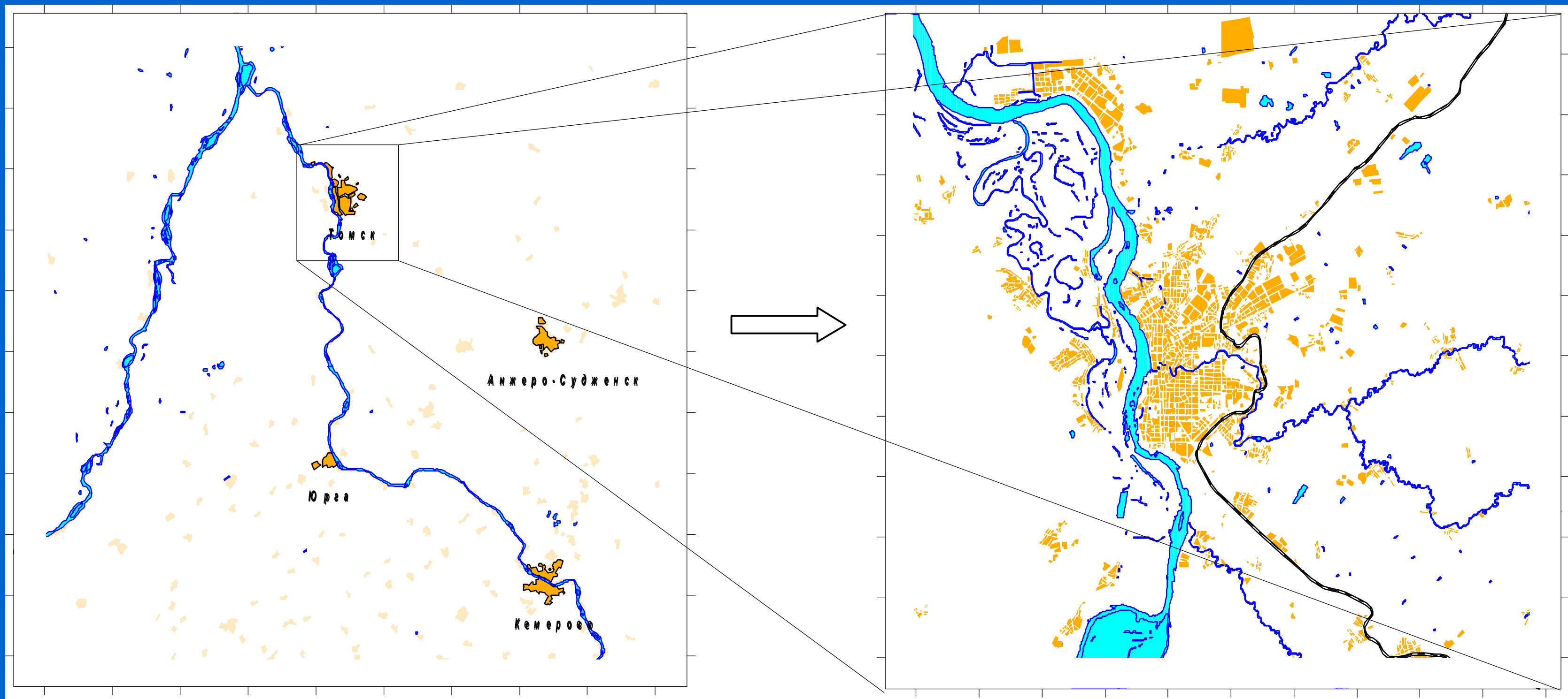
Numerical nonhydrostatic model

Terrain following (zeta) coordinate system
Nonhydrostatic hydrodynamic 3D equations
3D equations of heat and humidity exchange
Two-equation “k-l” turbulence model
2D equation for surface temperature
Assimilation of observed data
Nesting technology

Pollution transport model

Eulerian 3D equations for basic anthropogenic pollutants of near surface layer (dust, CO, SO_2, NO_2)
Dry deposition (resistance model)
Photochemical reactions of Hurley's GRS-mechanism of troposphere ozone and PM10 generation (CSIRO)
Data base of distributed point, area, mobile (linear) sources

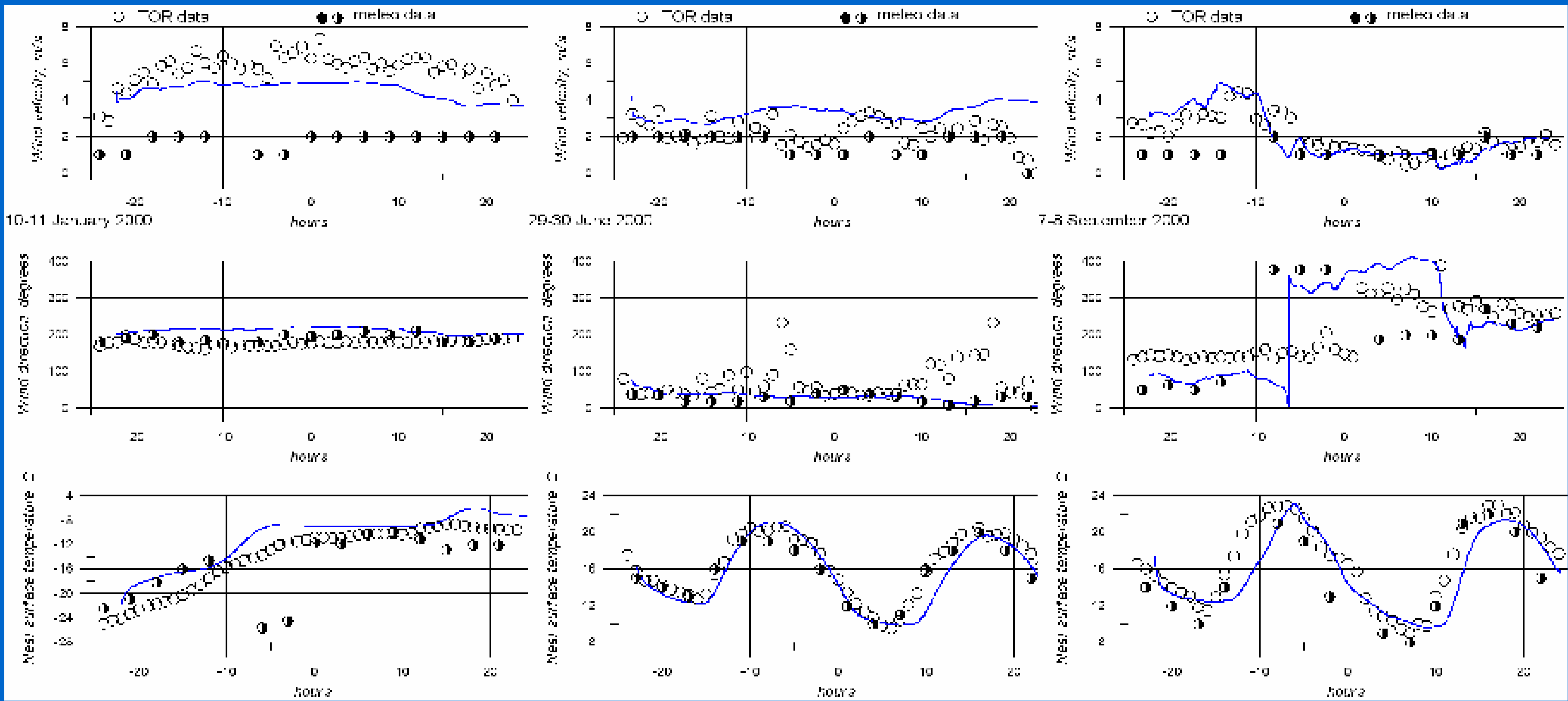
Nesting technology



Tomsk Region — Domain 200x200km^2

Tomsk City — Domain 50x50 km^2

Comparison of the predictions and the observed data



Meteodata of the IOA TOR-station and the Hydrometeorological Center

Comparison of MEMO and MS TSU-IOA predictio

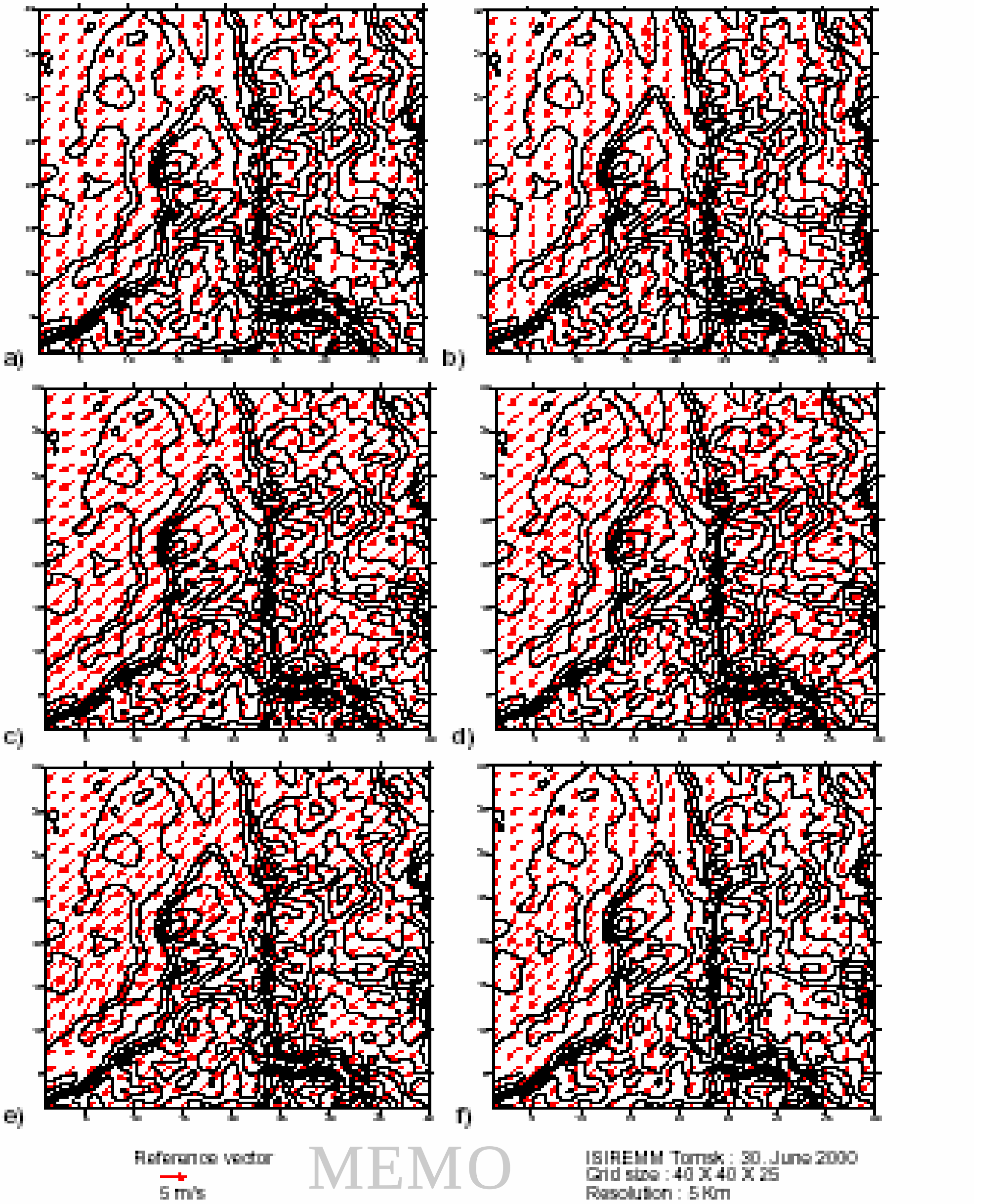
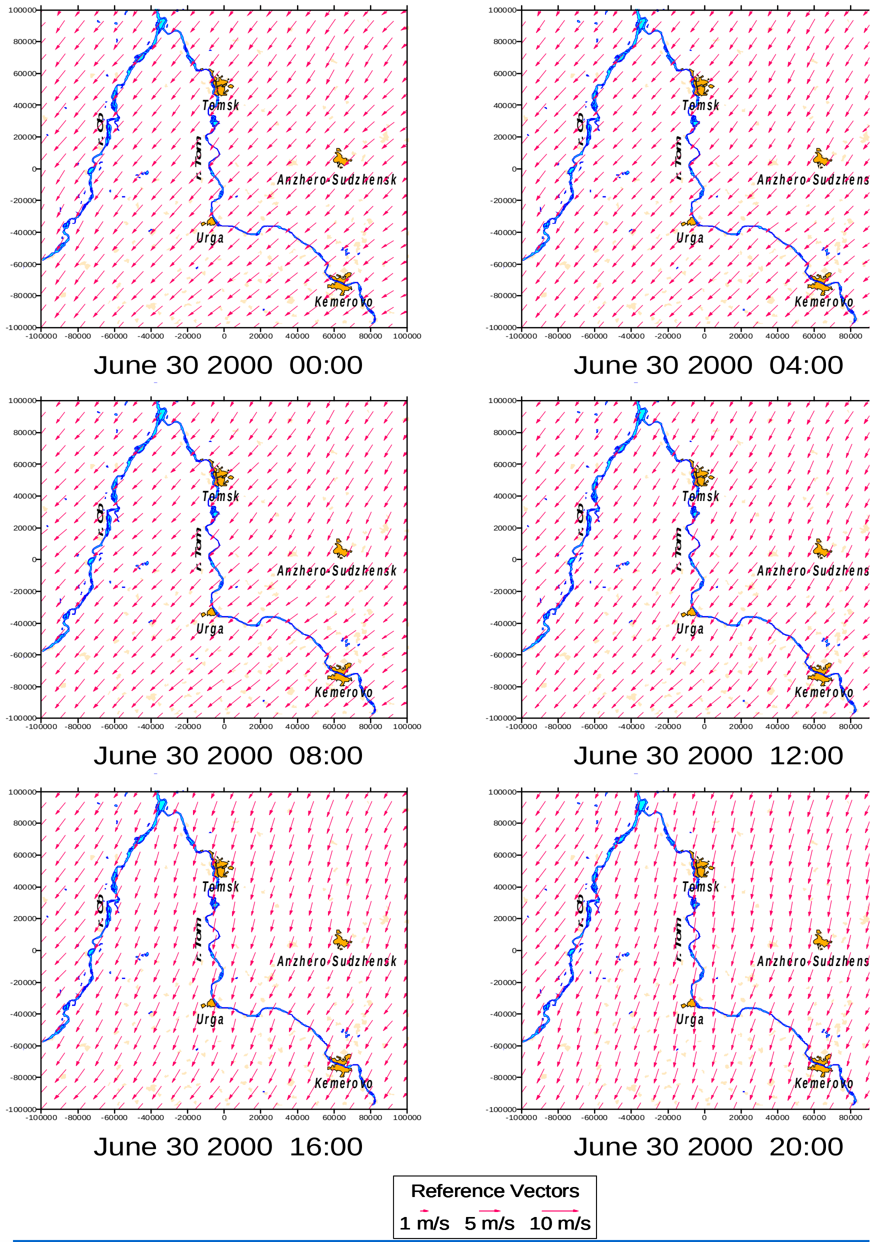
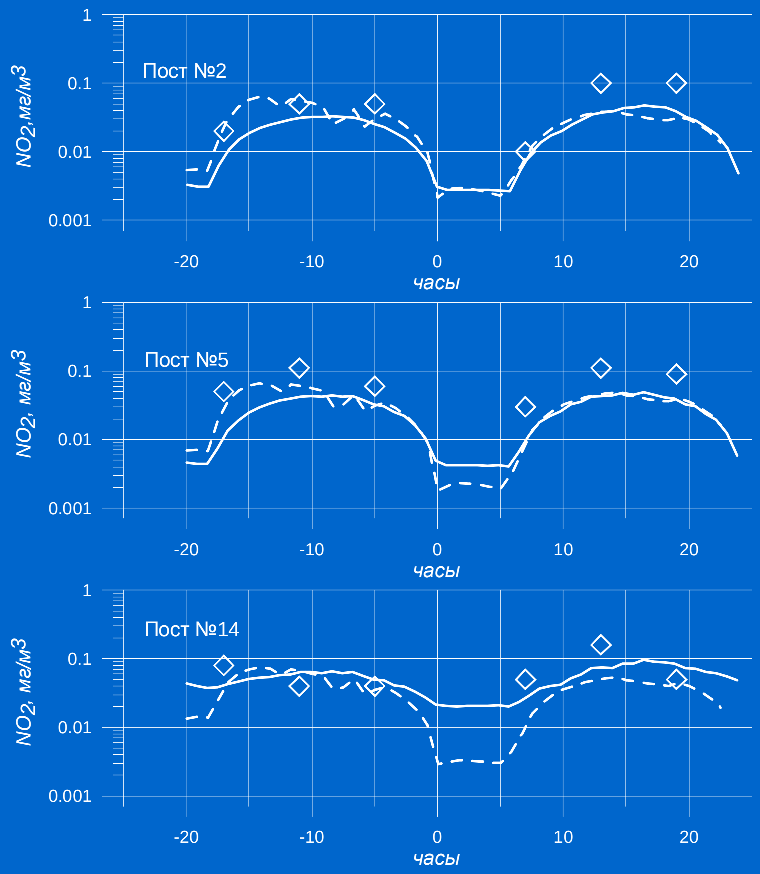


Fig. 10. Ground level wind field simulation results for the Tomsk Oblast area and for scenario B (30 June 2000): a) 0:00, b) 4:00, c) 8:00, d) 12:00, e) 16:00 and f) 20:00 (time in LST).



Prediction of pollutant concentrations in Tomsk



10-11 January 2000

3 inert pollutants: CO, SO_2, NO_2

Point and area sources

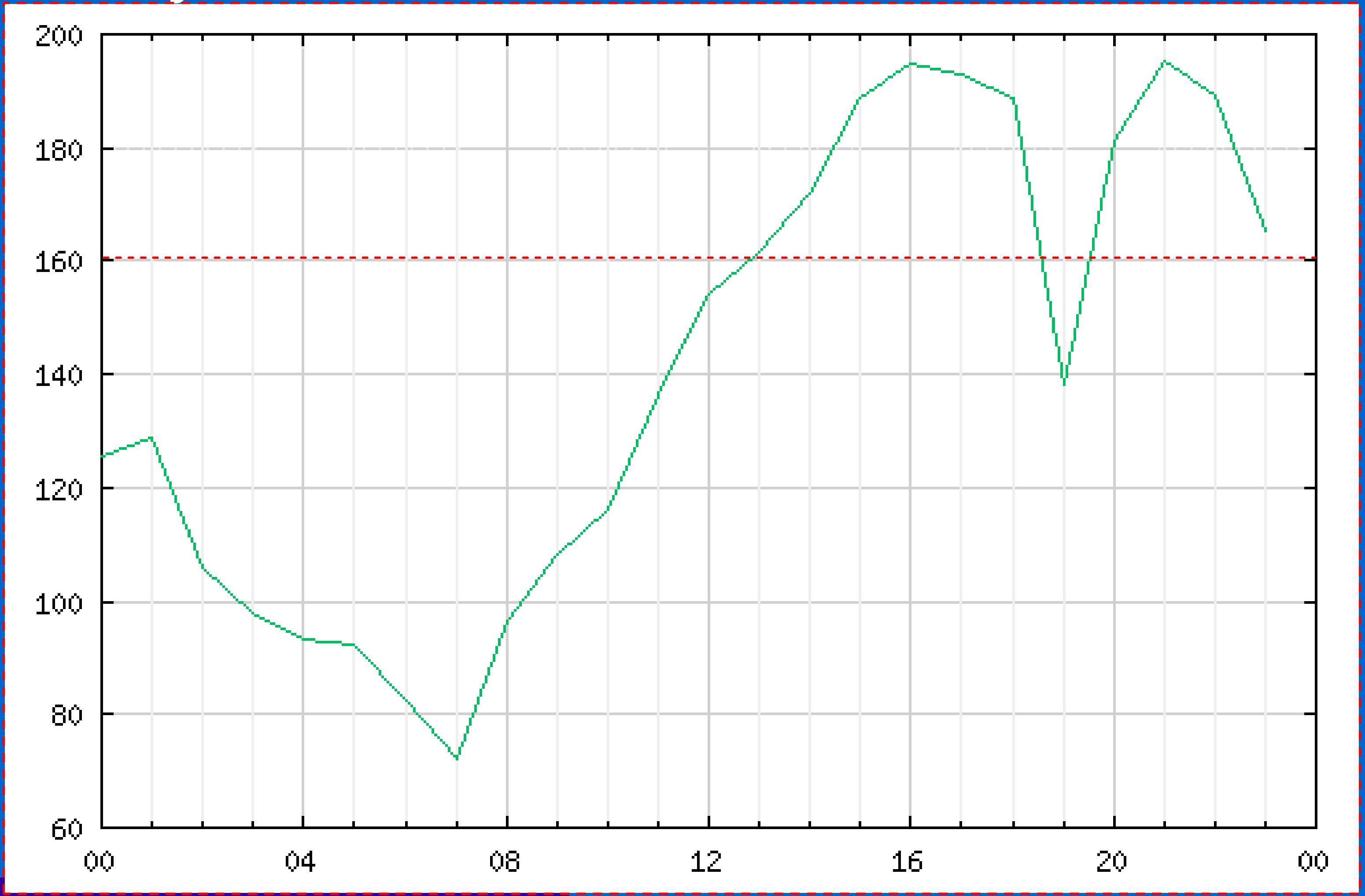
Emission rate of line sources:

$Q(h)=Qave*(0.1+1.9*\sin(\pi(h-6)/18)$, $6<h<24$ hours

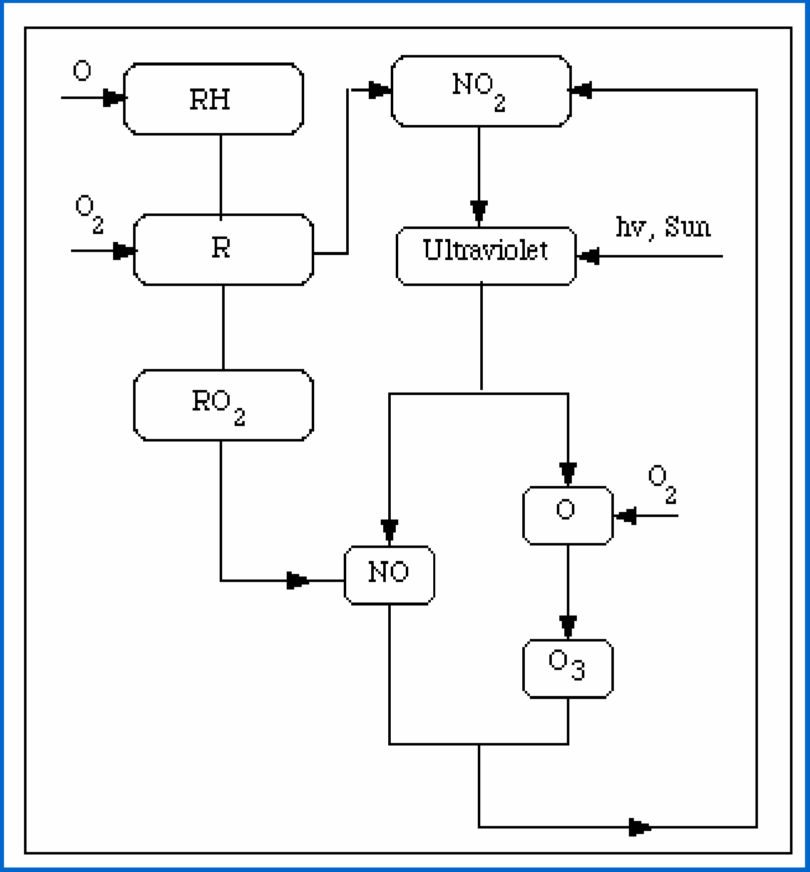
Computation grid: 100x100x60

Ozone concentration, observed in TOR-station IAO near Tomsk on 16 May 2004

O3, mkg/m^3

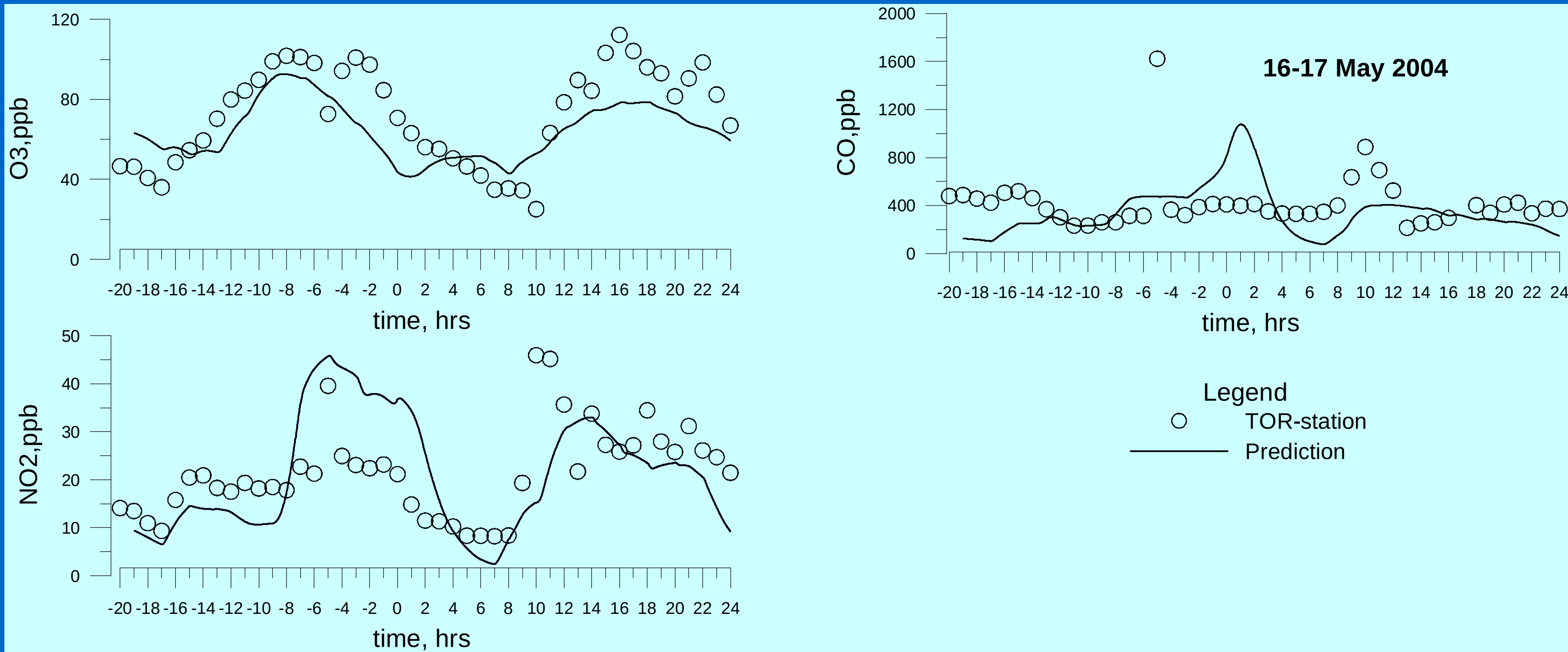


Generic Reaction Set kinetic scheme of ozone formation (Hurley,1999)



Rsmog + hv => RP + Rsmog + ηAPM
RP + NO => NO2
NO2 + hv => NO + O3
NO + O3 => NO2
RP + RP => RP + αH2O2
RP + NO2 => SGN
RP + NO2 => APM
RP + SO2 => APM
H2O2 + SO2 => APM
O3 + SO2 => APM

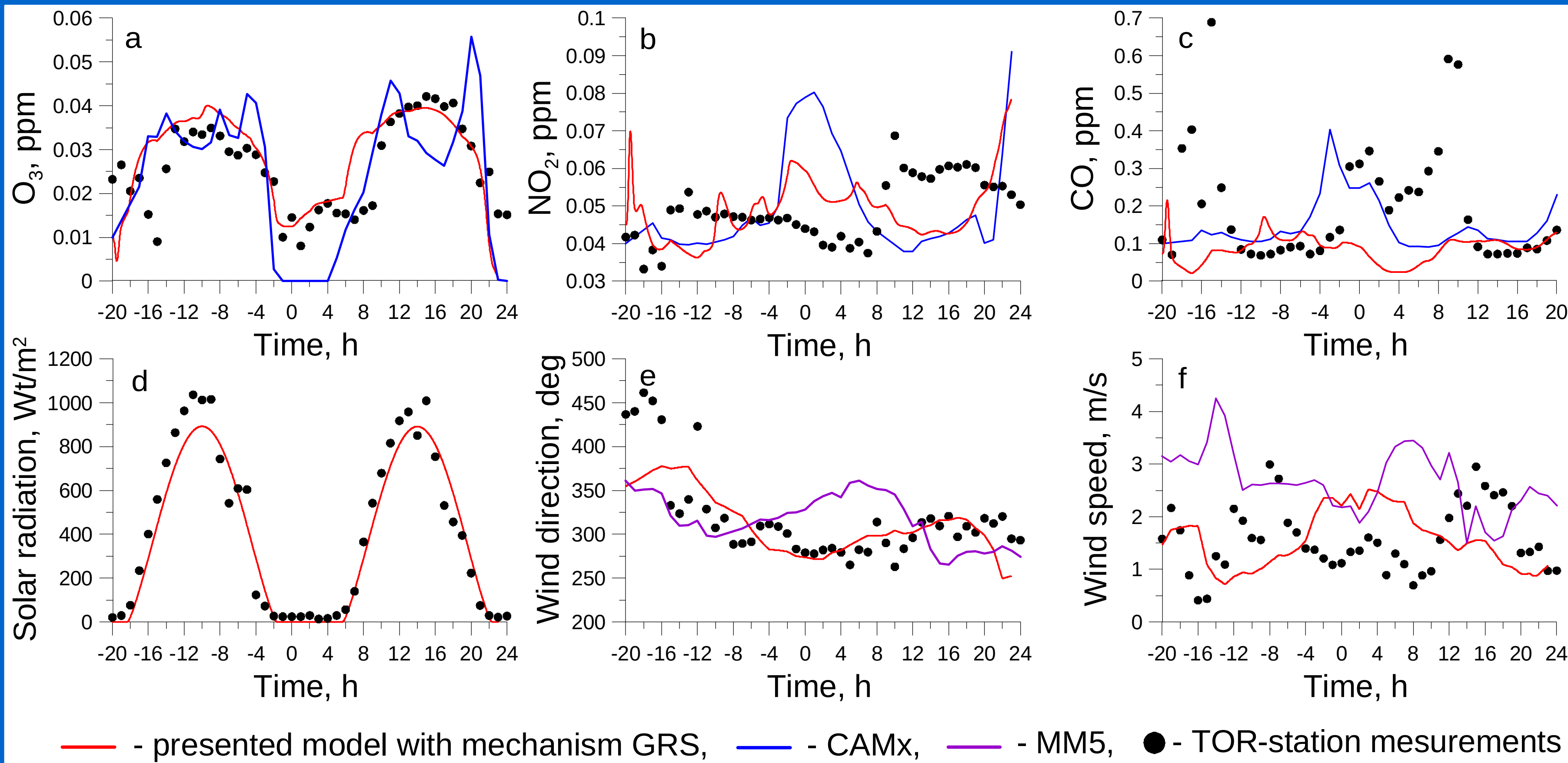
Air pollution in Tomsk



Time=-20…0: 16 May 2004;
Time= 0…24: 17 May 2004

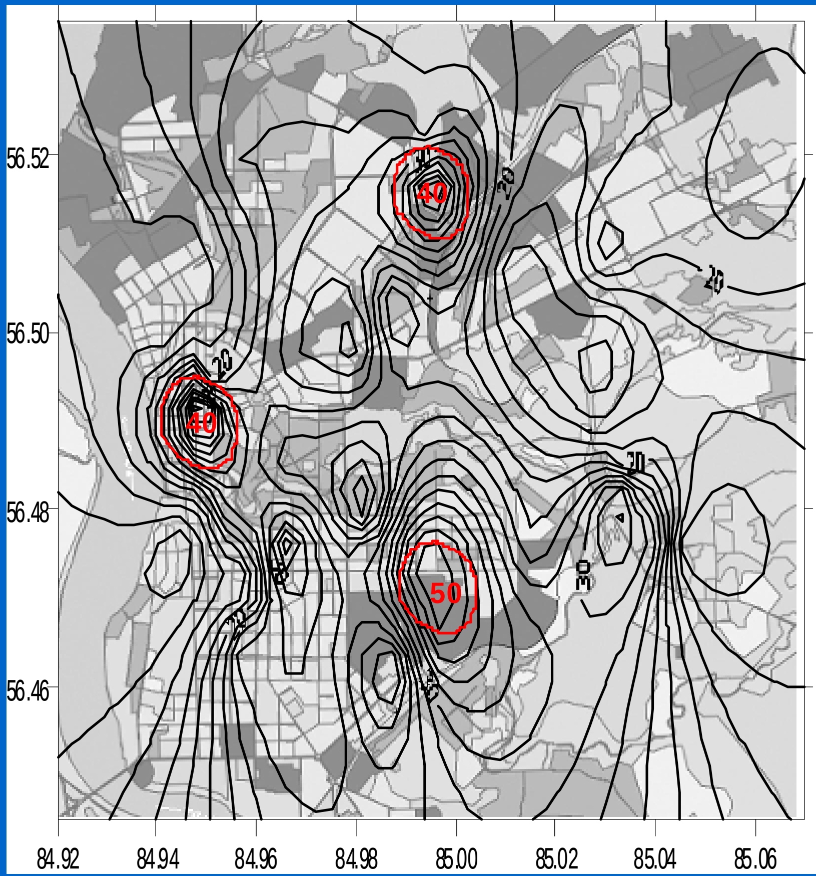
CAMx vs TSU-IAO MS

26-27 May 2004 in Tomsk

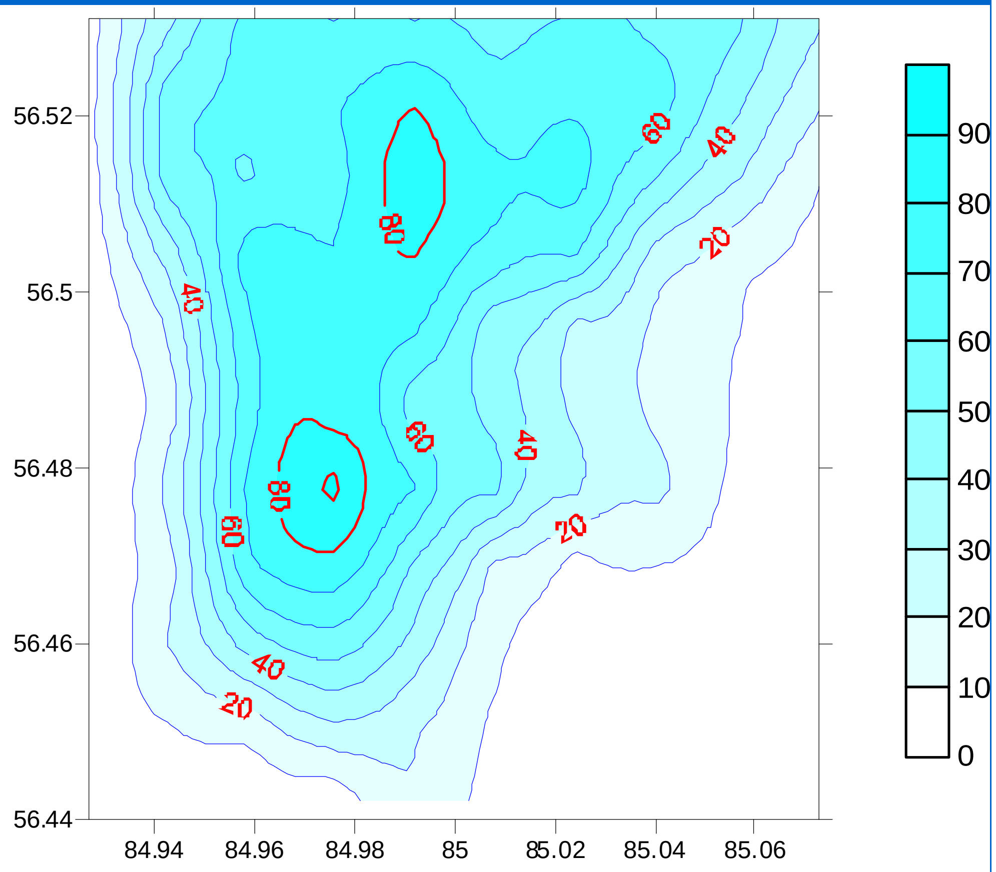


Результаты расчетов

Near surface concentration of nitrogen dioxide at 16:00 on 11 July 2005 in Tomsk



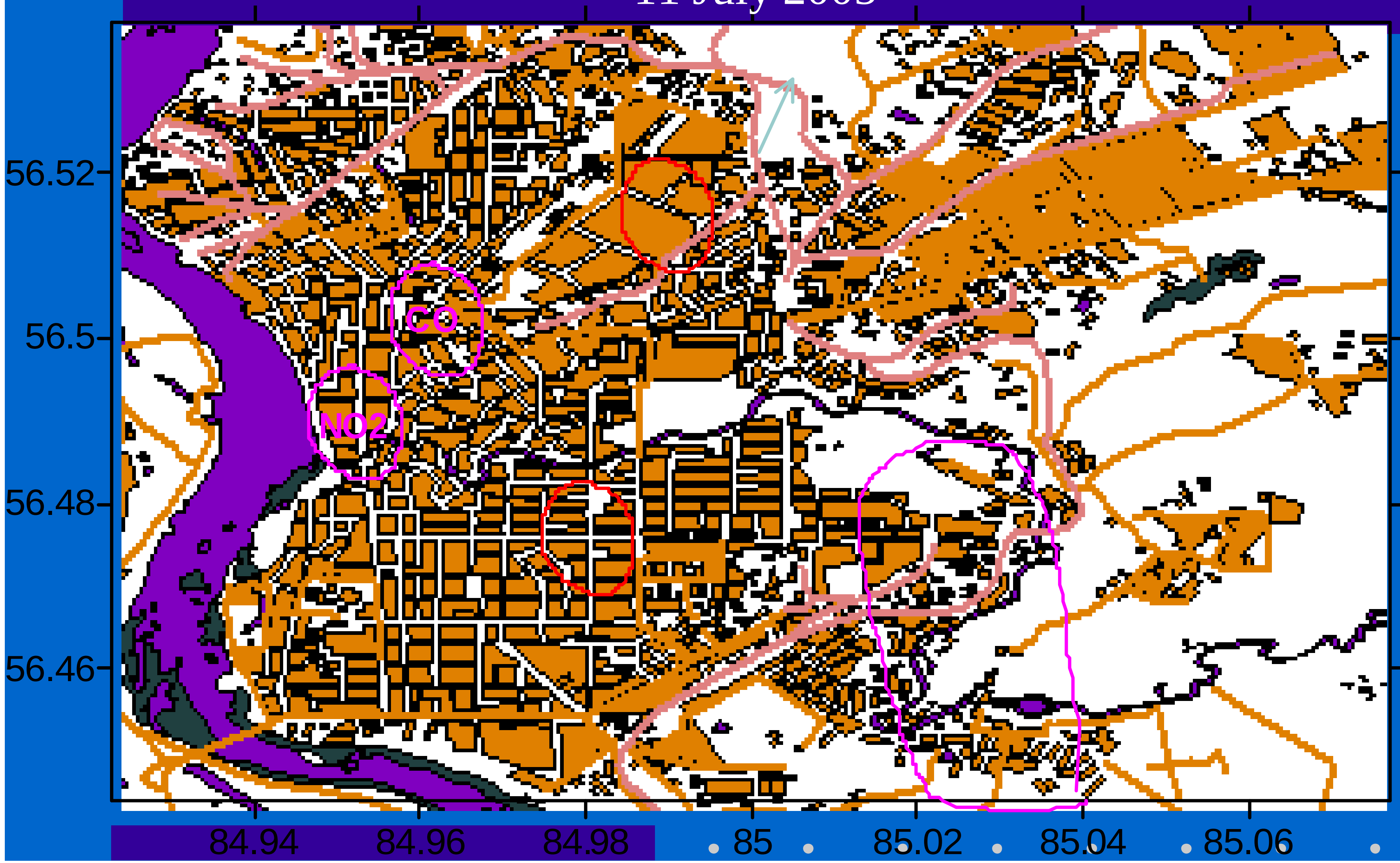
IAO Measurements



TSU-IAO MS Predictions

Results of AQ predictions in Tomsk

11 July 2005



Acknowledgements

This research is funded by RFBR,
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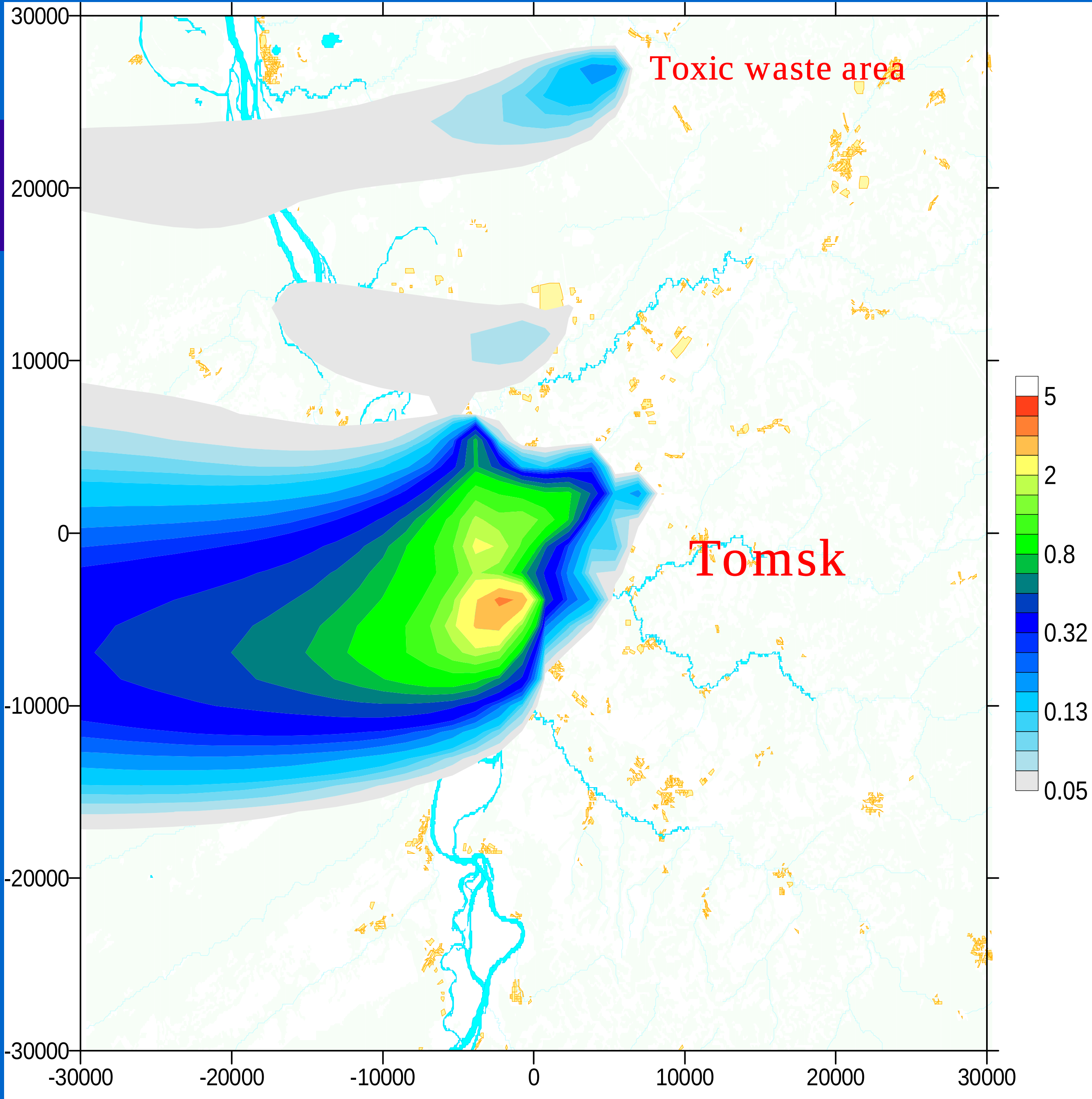
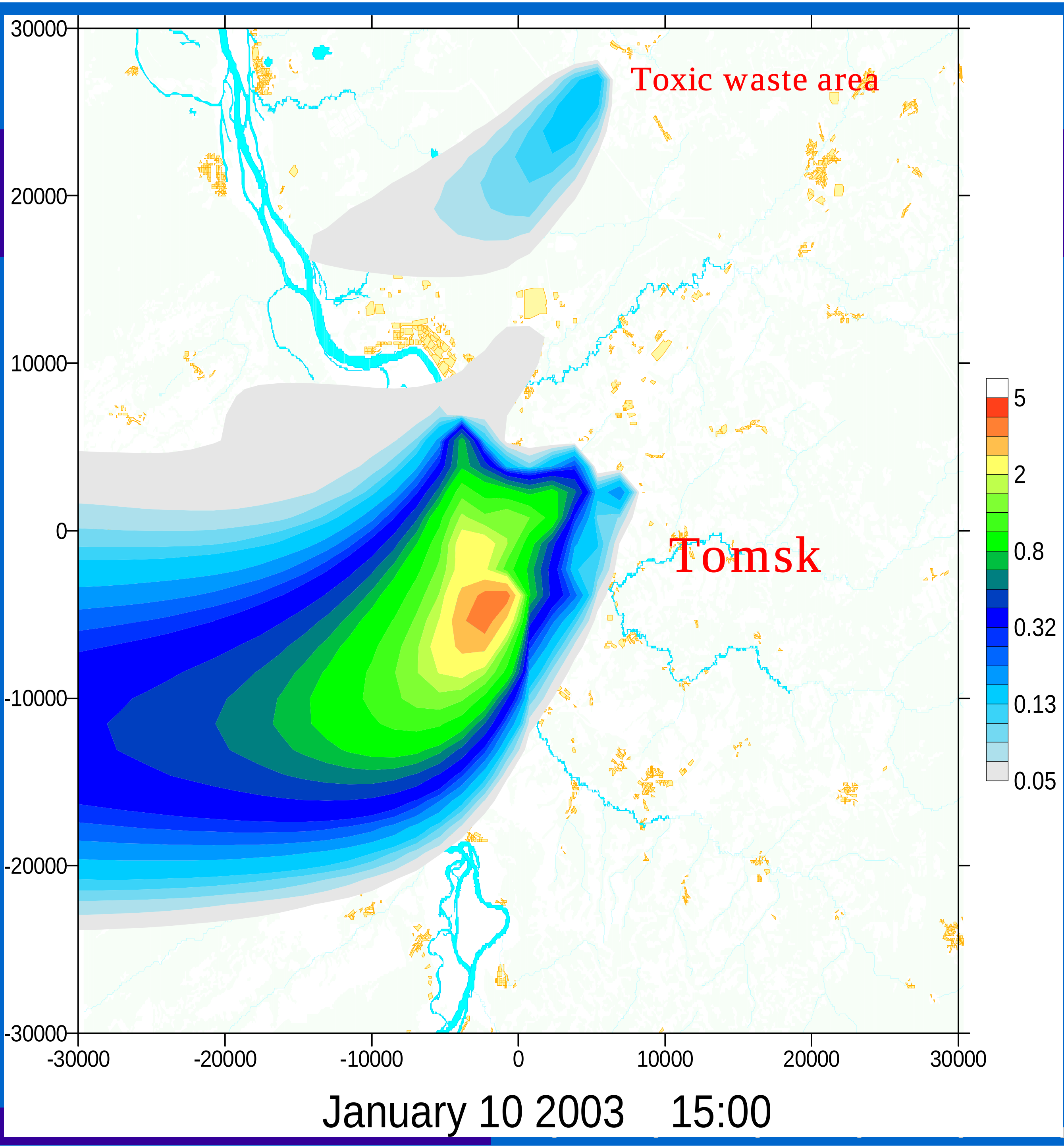
Fire in toxic waste area

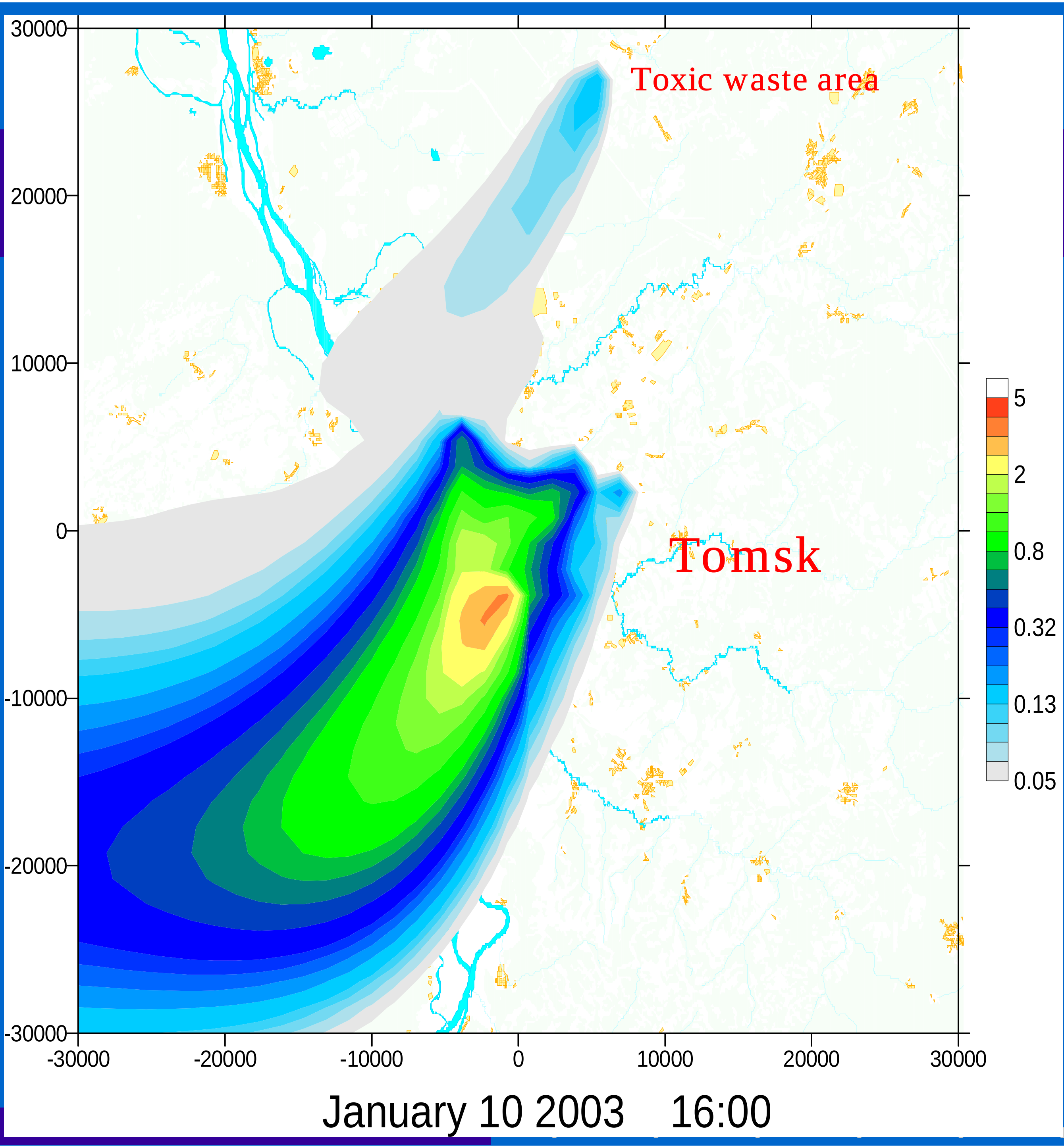
- 10 January 2003 fire was happened in the Tomsk area of toxic waste, located in the north of Tomsk.
- Conflagration duration was from 10.00 to 24.00.
- Inhabitants of Seversk, Svetly and Tomsk felt foxy smell.



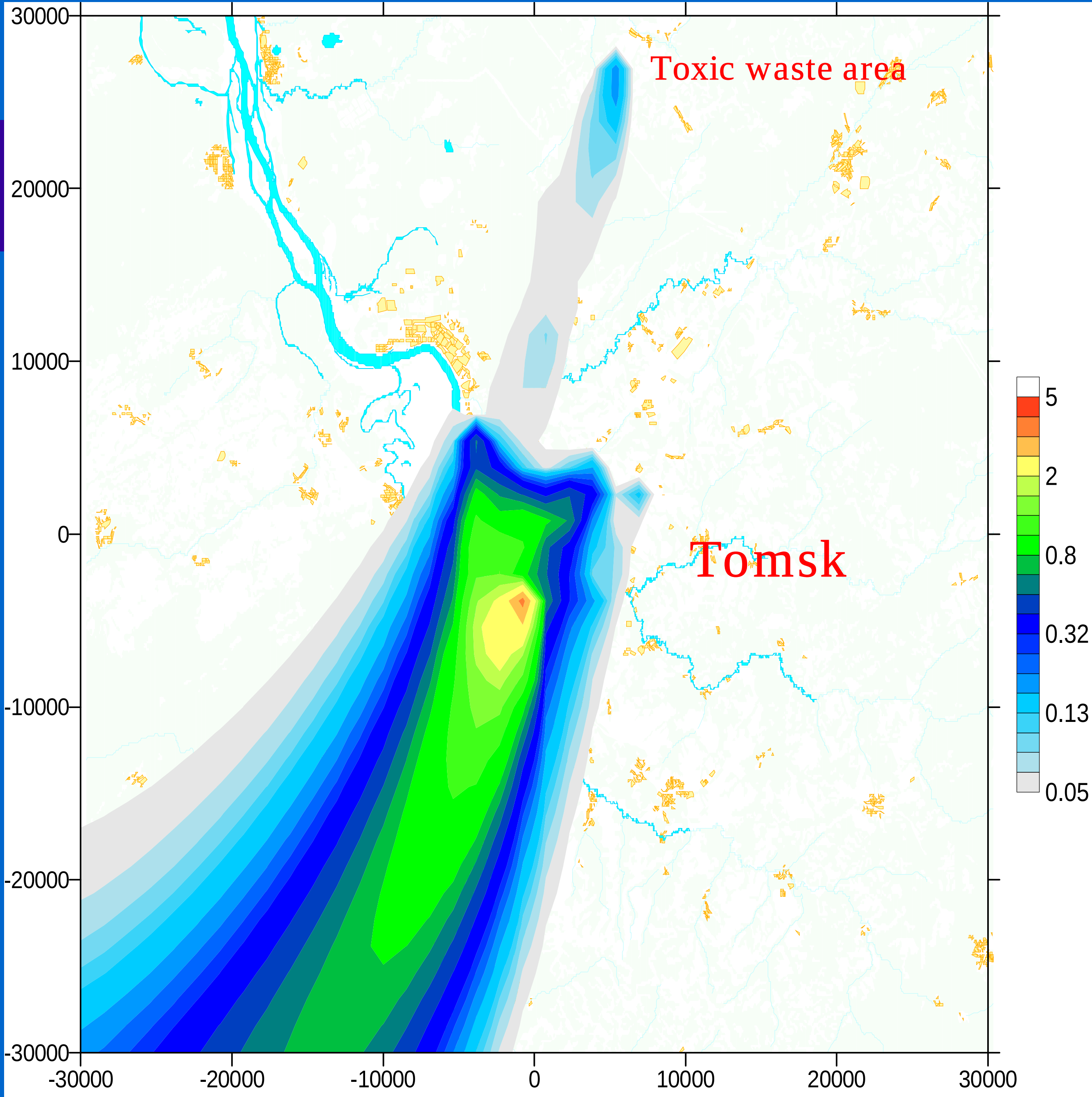
January 10 2003 14:00



Toxic waste area
Tomsk
30000
20000
10000
0
-10000
-20000
-30000
-30000
-20000
-10000
0
10000
20000
30000
5
2
0.8
0.32
0.13
0.05
January 10 2003 15:00



Toxic waste area
Tomsk
30000
20000
10000
0
-10000
-20000
-30000
-30000
-20000
-10000
0
10000
20000
30000
5
2
0.8
0.32
0.13
0.05
January 10 2003 16:00



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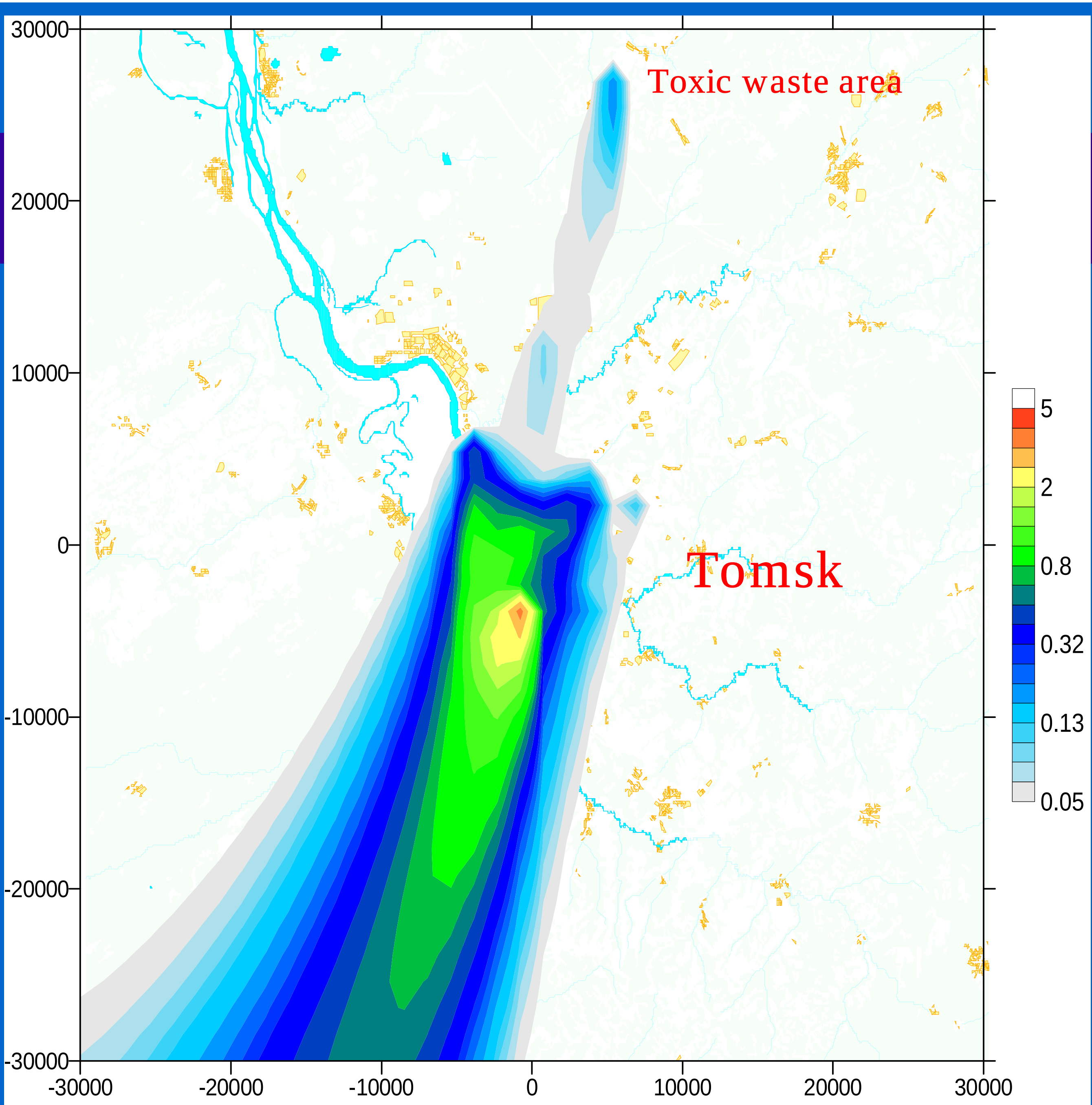

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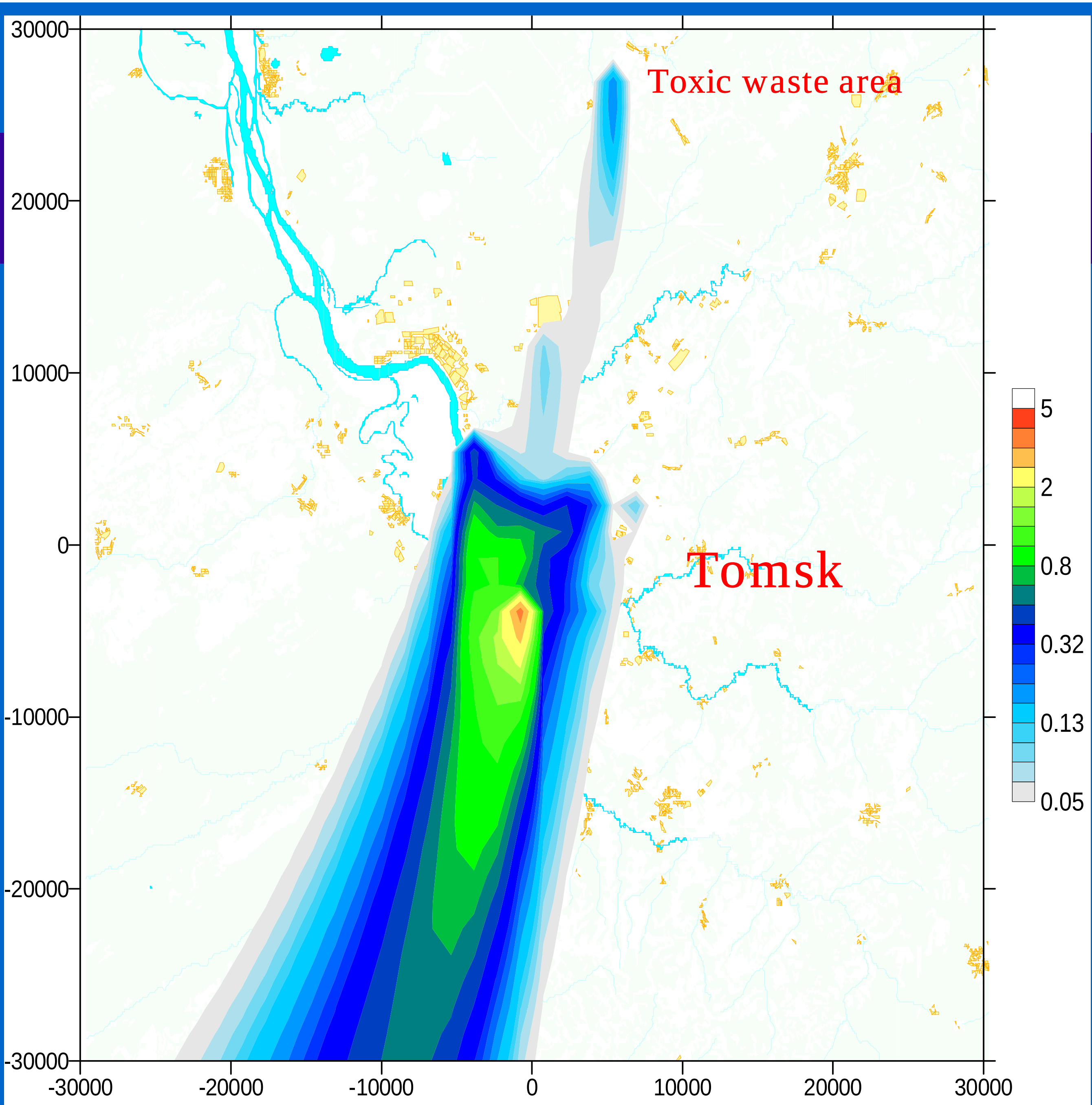

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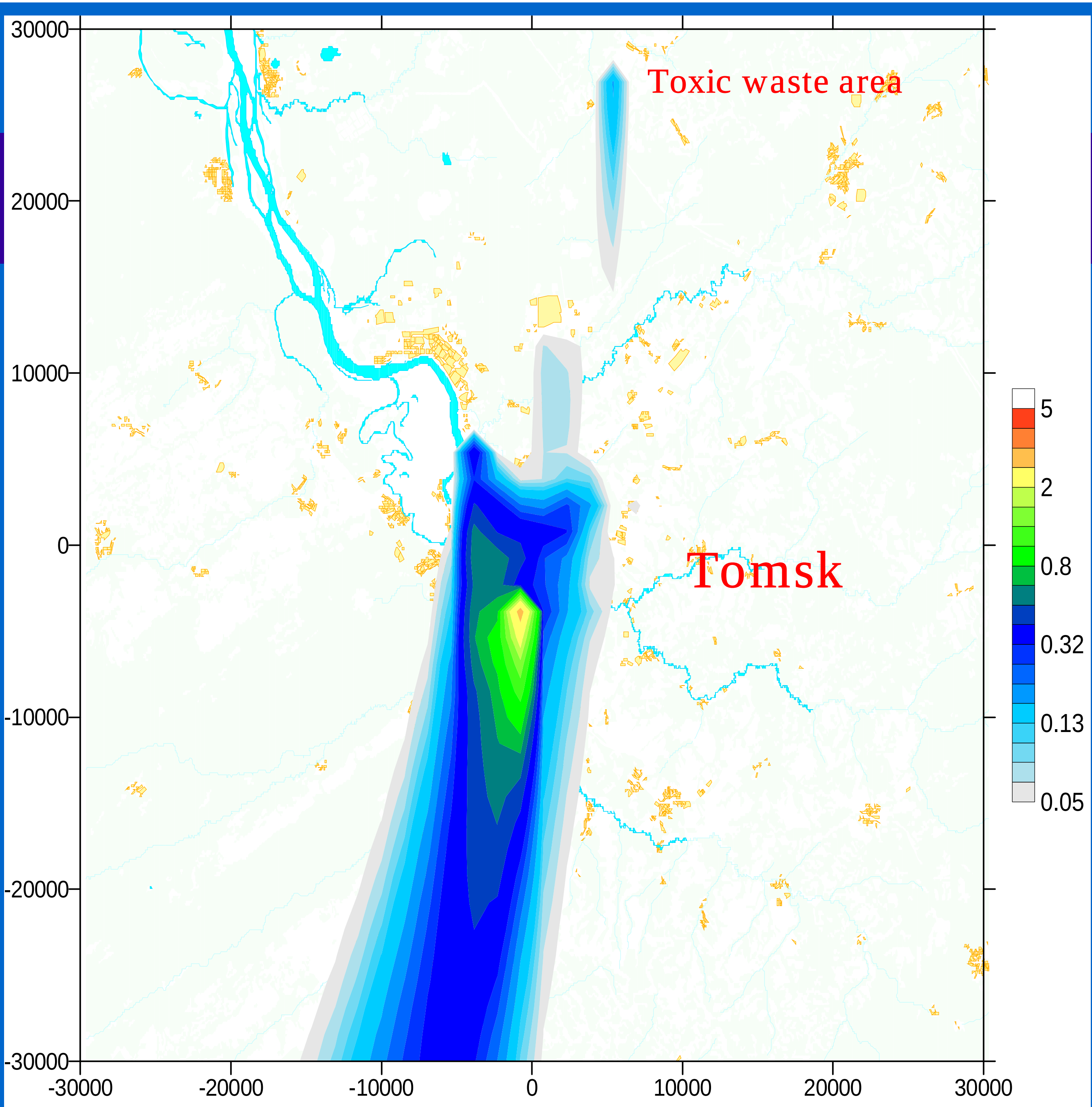

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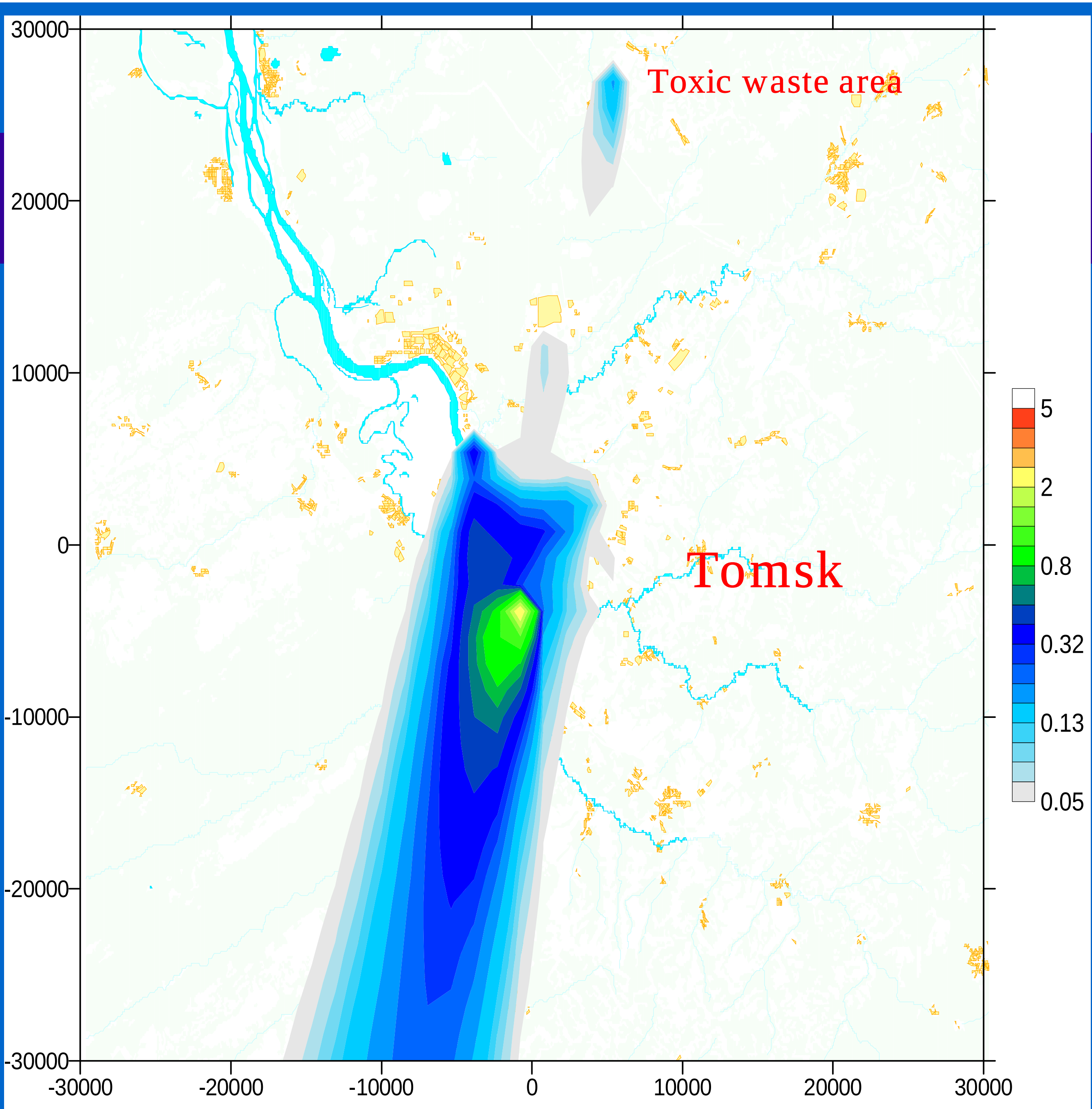
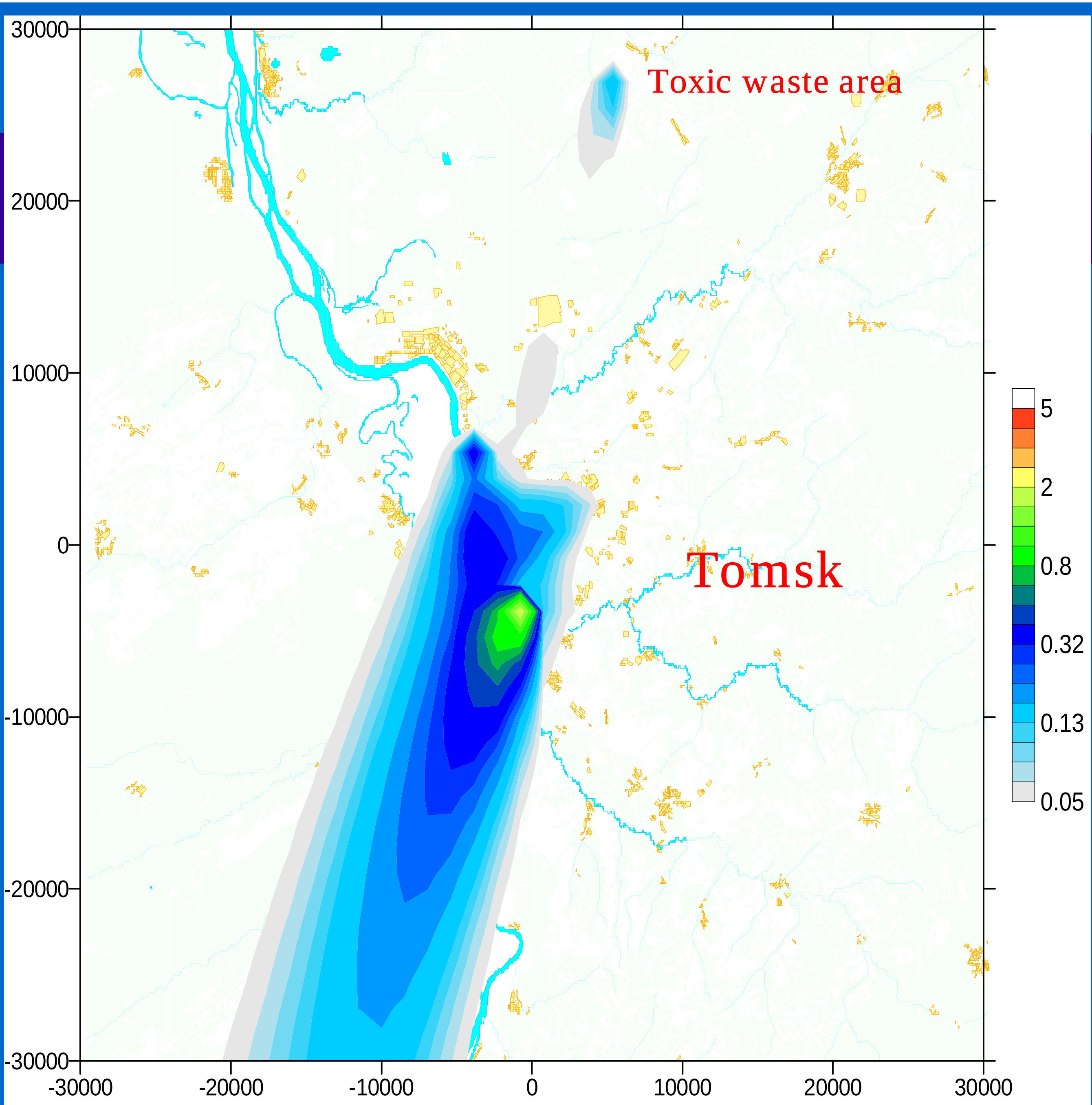


January 10 2003 23:00



January 11 2003 00:00