ACCENT/GLOREAM WORKSHOP
Berlin, Germany, 28-30 November 2007
Workshop on tropospheric chemical transport modeling

NUMERICAL SIMULATION OF AN EXTREME AIR POLLUTION EPISODE CREATED BY COAL BURNING THERMAL POWER PLANTS

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1. INTRODUCTION

- Several hot spots exist in Bulgaria
- Preliminary intention – Sofia or Burgas, motivation
- Final choice: Stara Zagora and the period of 8-11 July 2005, motivation

It have to be noticed that these pollution events caused big public complains and even political consequences. All this requires appropriate measures. However, to manage the situation is not trivial as the monitoring system (both emissions and ambient air concentrations) is not sufficient to explain the cases directly. Mathematical modeling is alternative tool according to the EU Framework Directive on Air Quality (96/62/ES) (see Skouloudis, 2005).

- Decription of the region:
  - big sity (300 000 habitants) and
  - powerful polluters near by.
- Description of “Maritza-Iztok” TPPs.

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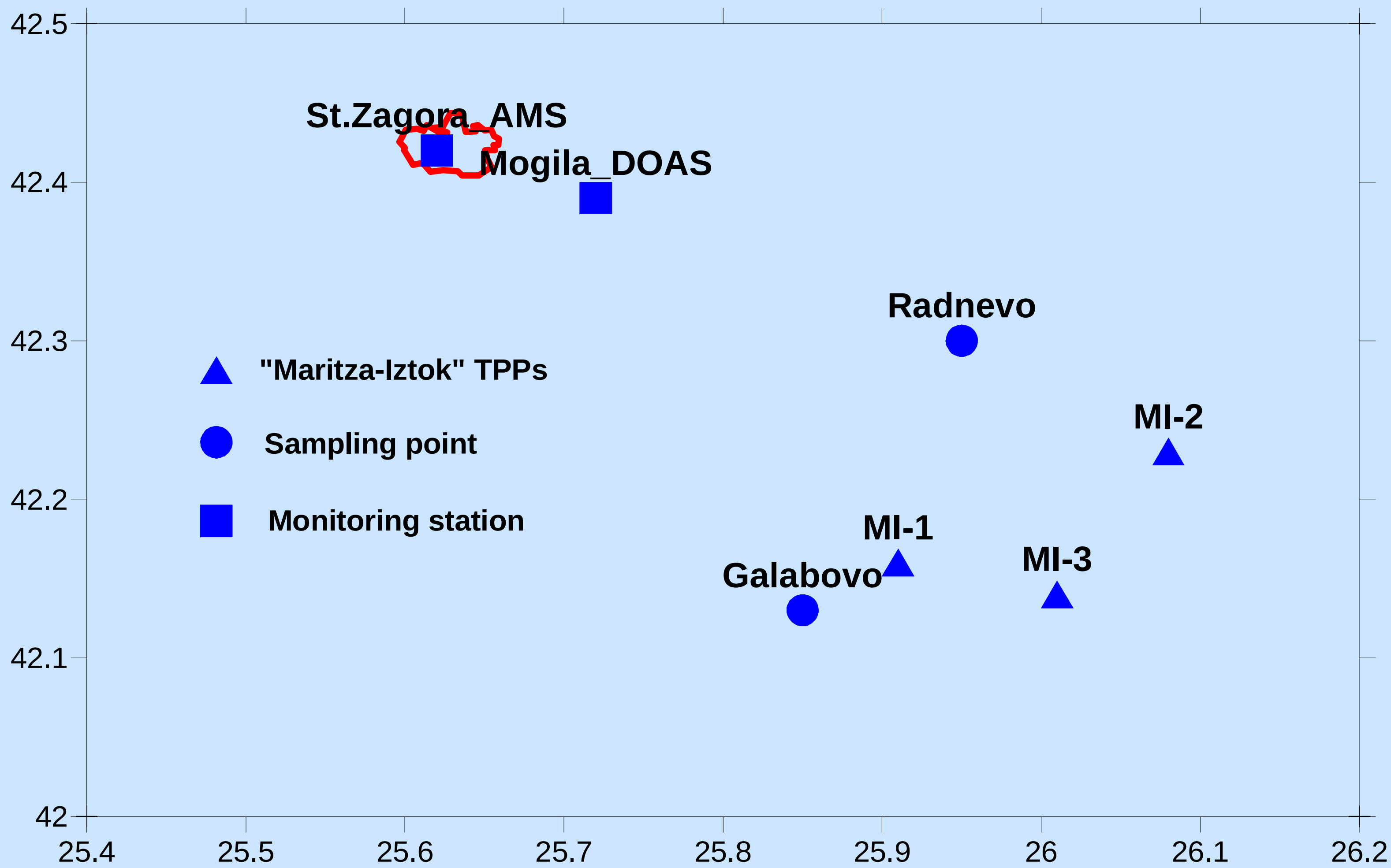

Configuration of Polluters and Receivers in the region of Stara Zagora

Emission parameters of “Maritza-Iztok” TPPs

TPP	Latitude	Longitude	Stack					SO_x, Mg	%
			N	height, m	Diameter, m	Temperature, ºC	Flow, Nm^3/h		
Maritza-Iztok 1	25.91	42.16	1	150	6	192	2116000	60139	6
Maritza-Iztok 2	26.08	42.23	1	325	12	192	5400000	310714	50
			2	325	10	178	2900000	173572	
Maritza-Iztok 3	26.01	42.14	1	325	12	192	5150000	156938	16
Total emitted								701363	72

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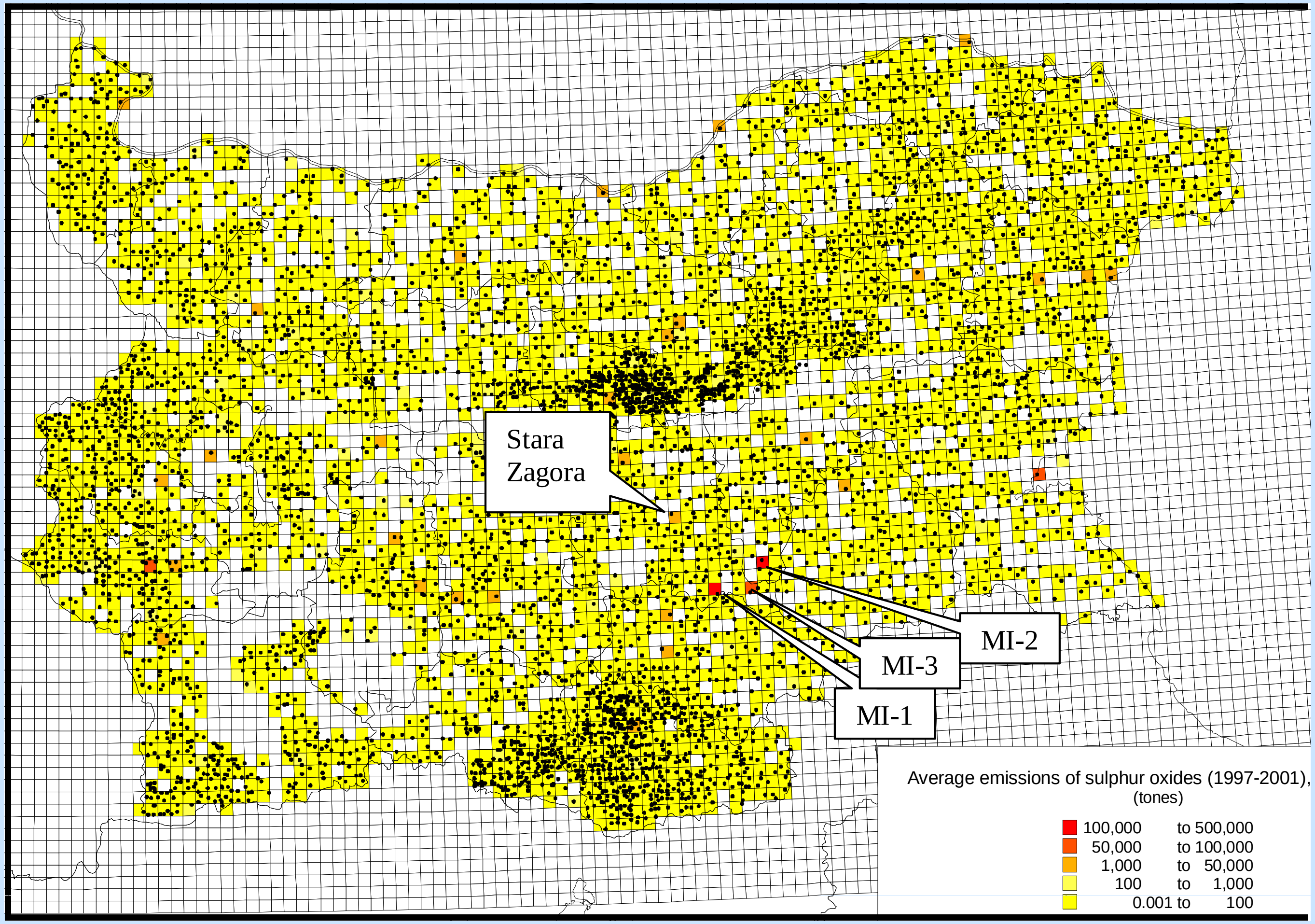

2. DESCRIPTION OF THE POLLUTION EPISODE

- 4 successive days
- very high SO_2 concentrations over Stara Zagora
- concentrations about and over the alert threshold (350 $\mu g/m^3$).
- in the afternoon hours
- appearance of mist and visibility decrease.

Keeping in mind that the high SO_2 pollution covered an area of several squared kilometers it is easy to estimate that tones of sulphur were released over the town.

As far as all this happened in summer time and the domestic heating can not be the reason for such pollution, the only sources can be the three TPPs disposed at 40 km southeast from the town.

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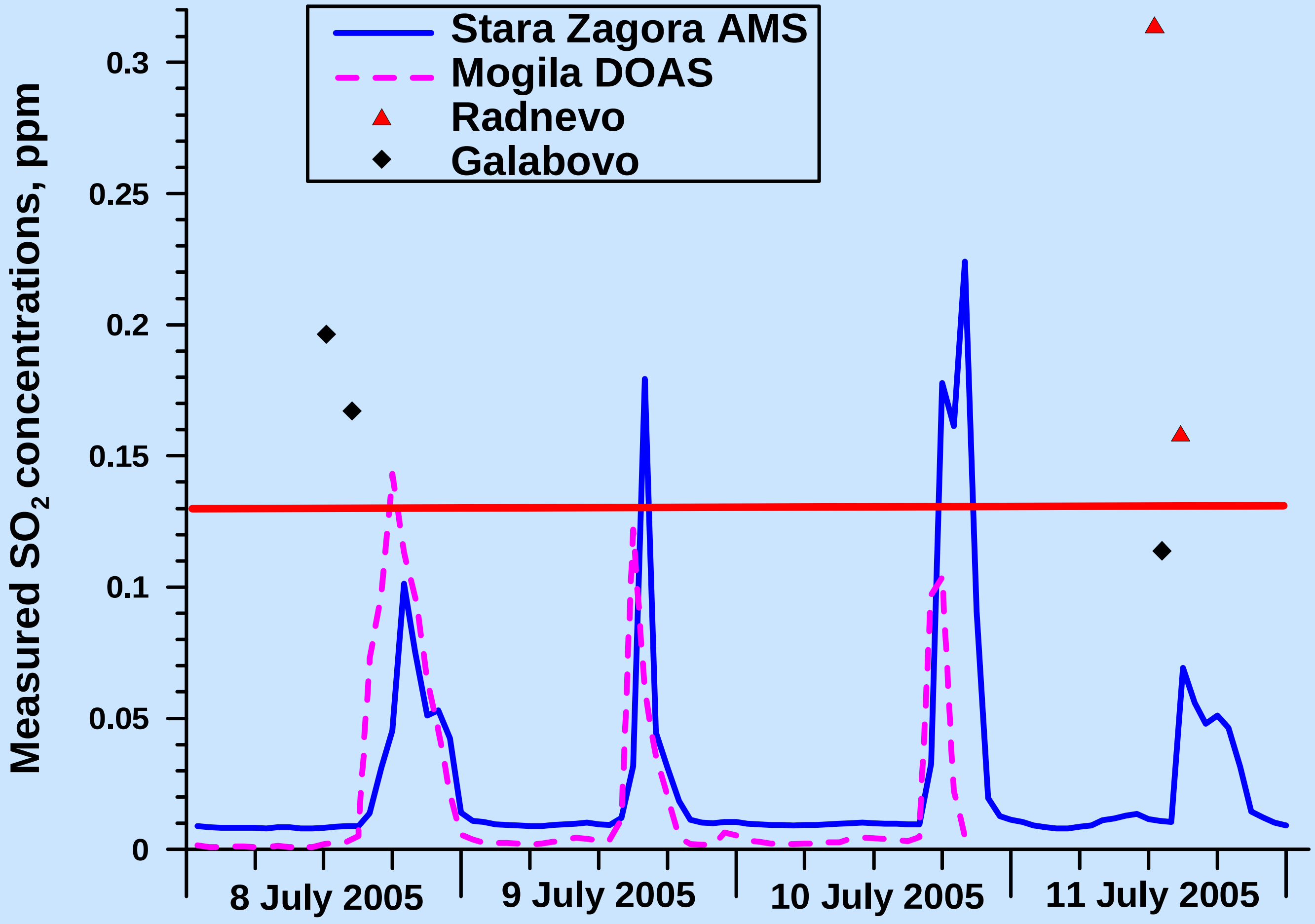

On a background of low SO_2 concentration (under 10 ppb) a sharp rise in concentration appear in the afternoon hours

On the base of physical considerations three possible mechanisms can explain this behavior:

1. In a stable PBL during the night and morning hours the plume from high stacks is keeping high SO_2 concentrations aloft some tens of kilometers from the sources. If a steady flow exists from southeast, such concentrations will exist over the Stara Zagora. The development of convective turbulence in the afternoon hours is dragging this pollution to the ground (fumigation). In the evening, the PBL gets stable and pollution does not influence the surface (see Palau et al., 2005, and their reference).

2. Meandering of the plume and the wind in the PBL changes its direction with time.

3. Combination of both mechanisms.

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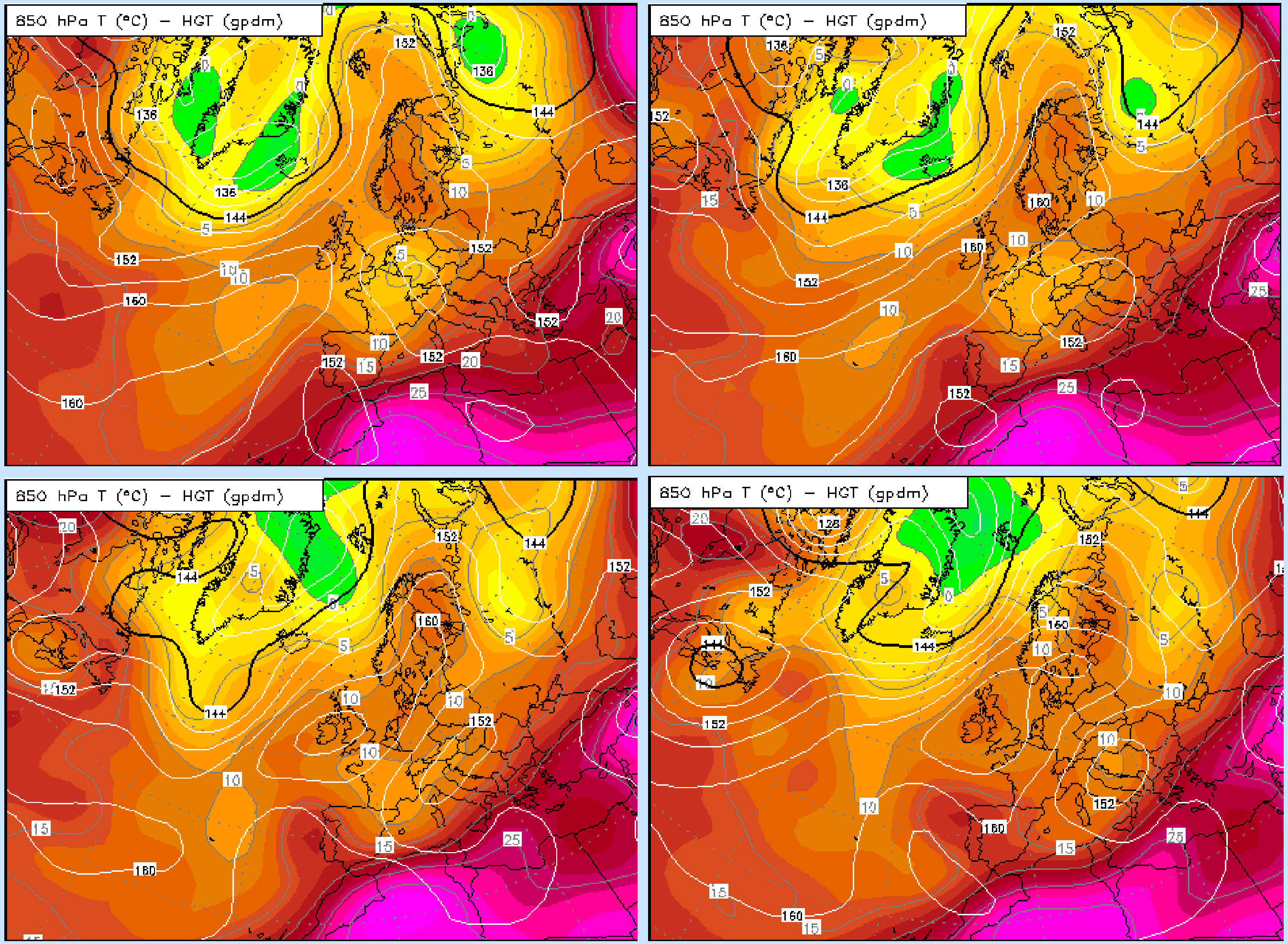
GLOREAM Modelling

3. WEATHER CONDITIONS DURING THE EPISODE

a) Synoptic situation over Europe in the period 8-11 July 2005



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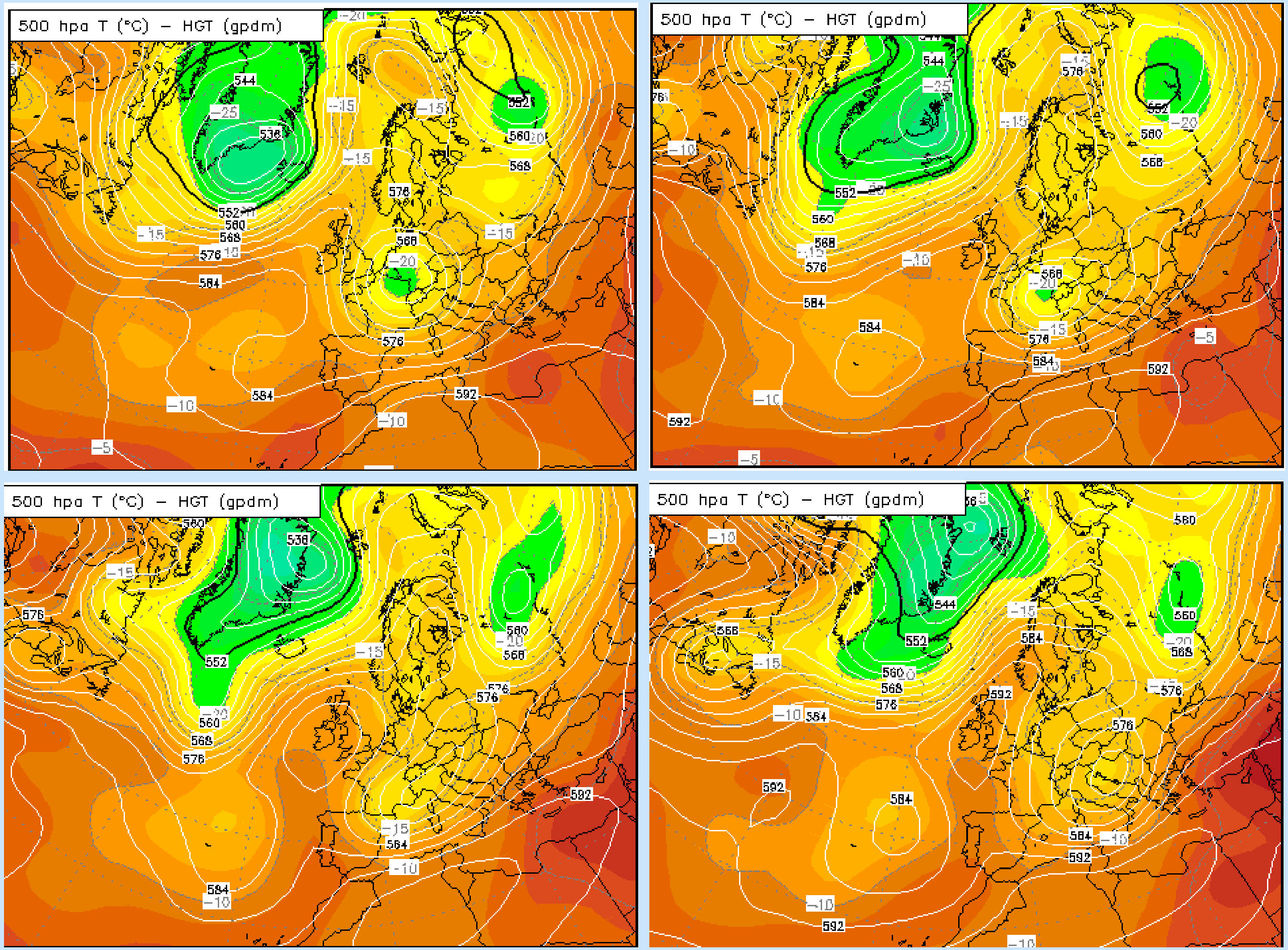

b) Characterization of the weather in Stara Zagora during the period

Day \ Hour	00 GMT	03 GMT	06 GMT	09 GMT	12 GMT	15 GMT	18 GMT
8.07.2005	14° calm	13° calm	17° SE, 2m/s	20° SE, 2m/s	25° SE, 2m/s	25° E, 2m/s	26° SE, 1m/s
9.07.2005	19° N, 2m/s	19° NE, 1m/s	21° calm	25° SE, 2m/s	28° SE, 5m/s	28° E, 5m/s	26° NE, 1m/s
10.07.2005	20° NE, 1m/s	18° NNE, 1m/s	21° calm	25° calm	28° SE, 5m/s	28° SE, 5m/s	26° calm
11.07.2005	19°, 1mm NE, 1m/s	17° calm	21° NW, 1m/s	26° W, 2m/s	29° SE, 5 m/s	24° calm	24°, 1mm calm

4. US EPA MODELS-3 SYSTEM

5th FP project BULAIR (http://www.meteo.bg/bulair)

- **Extensive review of the existing models and choice of a suitable modeling tool (availability, resources needed, completeness)**
- **Creation of respective data bases: meteorology, emissions, air quality, land-use etc.**
- **Studding and implementing the chosen model to different tasks**

Sources of information about models:

European MDS: air-climate.eionet.eu.int/databases/MDS/index_html

US EPA www.epa.gov/scram001/tt22.htm#rec

Choice of tool: Presentations to the last NATO/CCMS International Technical Meeting (ITM) on Air Pollution Modelling and Its Application

CMAQ	26th ITM, Turkey, May 2003	27th ITM, Canada, Oct 2004	28th ITM, Germany, May 2006
# present	9	17	40

It can be seen that CMAQ is implemented with increasing intensity. This model is a part of the lastly created US EPA Models-3 system.

The US EPA Models-3 system consists of:

- **the Community Multiscale Air Quality System CMAQ**
- **the 5th generation PSU/NCAR Meso-meteorological Model MM5**
- **the Sparse Matrix Operator Kernel Emissions Modeling System SMOKE**

This system and its parts appear to be ones of the most widely used models.

Important advantages: free downloadable, can be run on contemporary PCs.

This is a modeling tool of large flexibility with a range of options and possibilities to be used for different applications. Many research groups in USA and Europe not only use the Model-3 system or some of its elements but contribute to its further development.

5. DETERMINATION OF THE MODEL DOMAINS

- meteorology from NCEP Global Analysis Data for 2005 exploited.
- space resolution 1º×1º (i.e. ~100 km)
- MM5 nesting capabilities used, program TERRAIN
- 5 nested domains
- USGS global terrain and land use data sets are exploited

Domain	D1	D2	D3	D4	D5
Resolution, km	81	27	9	3	1
points	37×37	55×55	46×55	37×37	55×55
USGS data Resolution, km	~ 56	~19	~9	~ 4	~ 0.9

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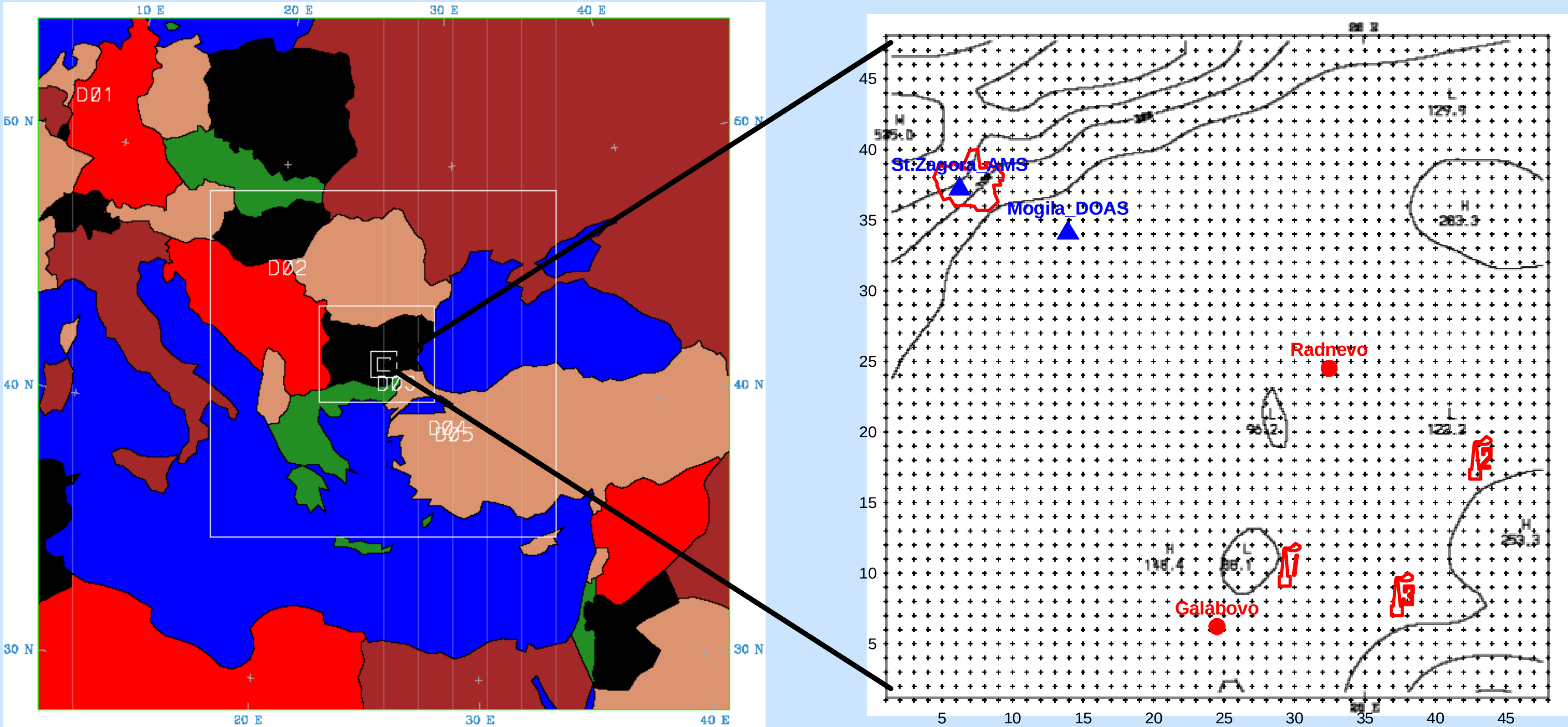

6. MM5 SIMULATIONS

MM5 is used to supply CMAQ with meteorological input.

As a hole, MM5 solves the non-hydrostatic system of dynamic weather equations in σ-coordinate system:

$$\frac{\partial u}{\partial t}+\frac{m}{\rho}\left(\frac{\partial p'}{\partial x}-\frac{\sigma}{p^*}\frac{\partial p^*}{\partial x}\frac{\partial p'}{\partial \sigma}\right)=-\mathbf{V}.\nabla u+v\left(f+u\frac{\partial m}{\partial y}-v\frac{\partial m}{\partial x}\right)-ew\cos\alpha-\frac{uw}{r_{earth}}+D_u$$

$$\frac{\partial v}{\partial t}+\frac{m}{\rho}\left(\frac{\partial p'}{\partial y}-\frac{\sigma}{p^*}\frac{\partial p^*}{\partial y}\frac{\partial p'}{\partial \sigma}\right)=-\mathbf{V}.\nabla u+u\left(f+u\frac{\partial m}{\partial y}-v\frac{\partial m}{\partial x}\right)-ew\sin\alpha-\frac{vw}{r_{earth}}+D_v$$

$$\frac{\partial w}{\partial t}+\frac{\rho_0}{\rho}\frac{g}{p^*}\frac{\partial p'}{\partial \sigma}+\frac{g}{\gamma}\frac{p'}{p}=-\mathbf{V}.\nabla w+g\frac{p_0}{p}\frac{T'}{T_0}-g\frac{p'}{p}\frac{R_d}{c_p}+e(u\cos\alpha-v\sin\alpha)-\frac{u^2+v^2}{r_{earth}}+D_w$$

$$\frac{\partial T}{\partial t}=-\mathbf{V}.\nabla T+\frac{1}{\rho c_p}\left(\frac{\partial p'}{\partial t}+\mathbf{V}.\nabla p'-\rho_0 gw\right)+\frac{Q}{c_p}+\frac{T_0}{\theta_0}D_\theta$$

$$\frac{\partial p'}{\partial t}-\rho_0 gw+\gamma p\nabla.\mathbf{V}=-\mathbf{V}.\nabla p'+\frac{\gamma p}{T}\left(\frac{Q}{c_p}+\frac{T_0}{\theta_0}D_\theta\right)$$

- **Nesting modes:**
  "two-way" nesting for D1 and D2
  "one-way" nesting for D3, D4 and D5 (separate runs)
- **Boundary conditions:**
  D1 – from NCEP data, FDDA option on
  D2 – from D1
  ……………..
  D5 – from D4
- **Vertical structure: 23 levels, 6 levels in PBL**

Level	0	1	2	3	4	5	6	7	...	23
sigma	1.00	0.99	0.98	0.96	0.93	0.89	0.85	0.80	...	0.00
pressure	1000	991	982	964	937	901	865	820	...	100
height, m	0	73	146	294	521	832	1153	1569	...	14662

- **Integration period: from 12:00 of 7 July 2005 to 00:00 of 12 July 2005**

ANALYSIS OF THE OBTAINED FIELD

PBL, where the dispersion of pollutants occurs, is complex and difficult to model in details (in time and space) over non-homogeneous terrain.

The MM5 system provides a number of combinations of different PBL parameterization schemes. The choice of appropriate scheme for a region is usually made by validation. Air temperature, humidity, wind speed and direction measurement data are needed for the purpose.

In the region of Stara Zagora no validation data are available for the vertical structure of atmosphere.

In the present simulation the lack of information for validation is clearly disturbing.

The modeled flows, here, are obtained by using the MRF PBL parameterization scheme.

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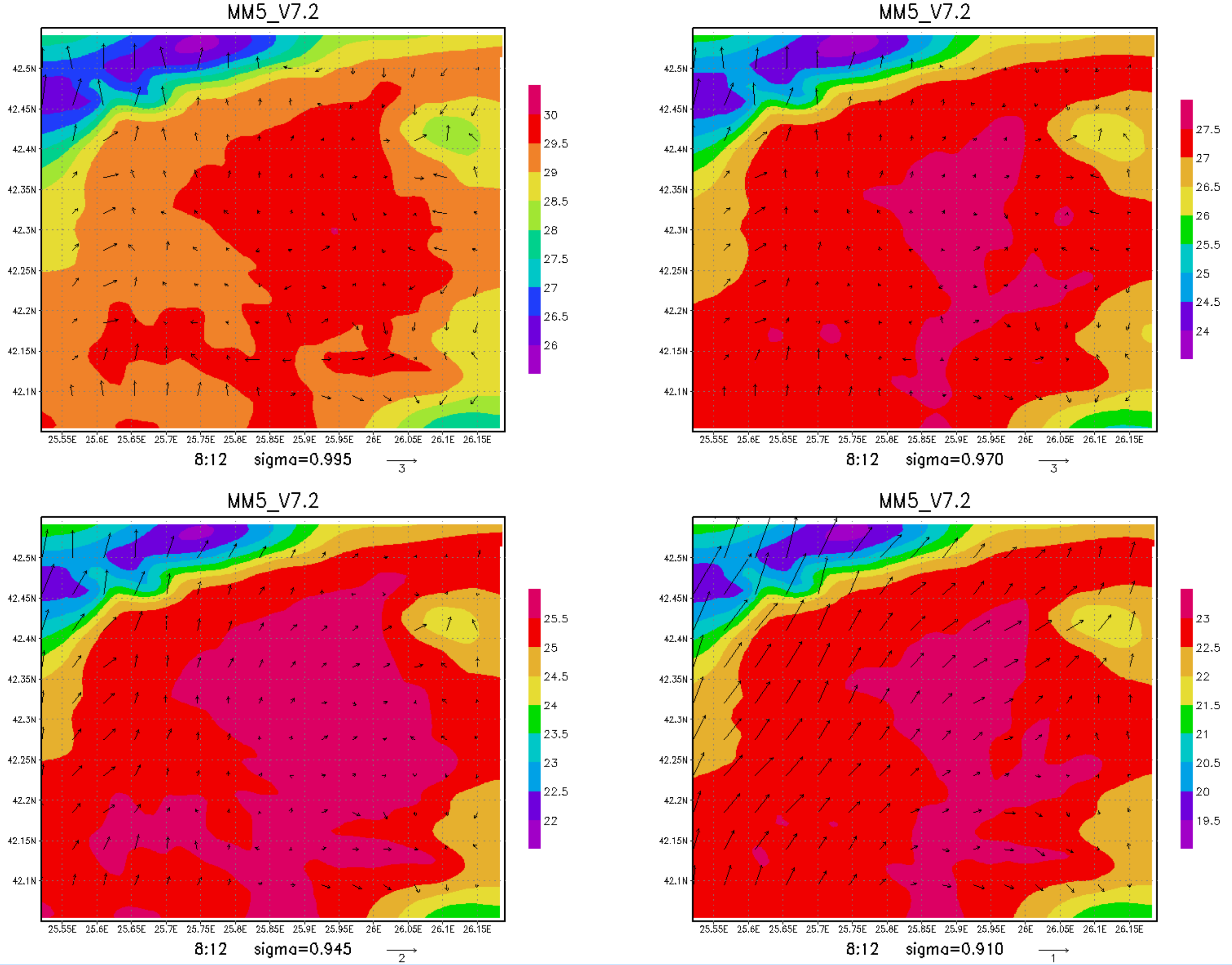

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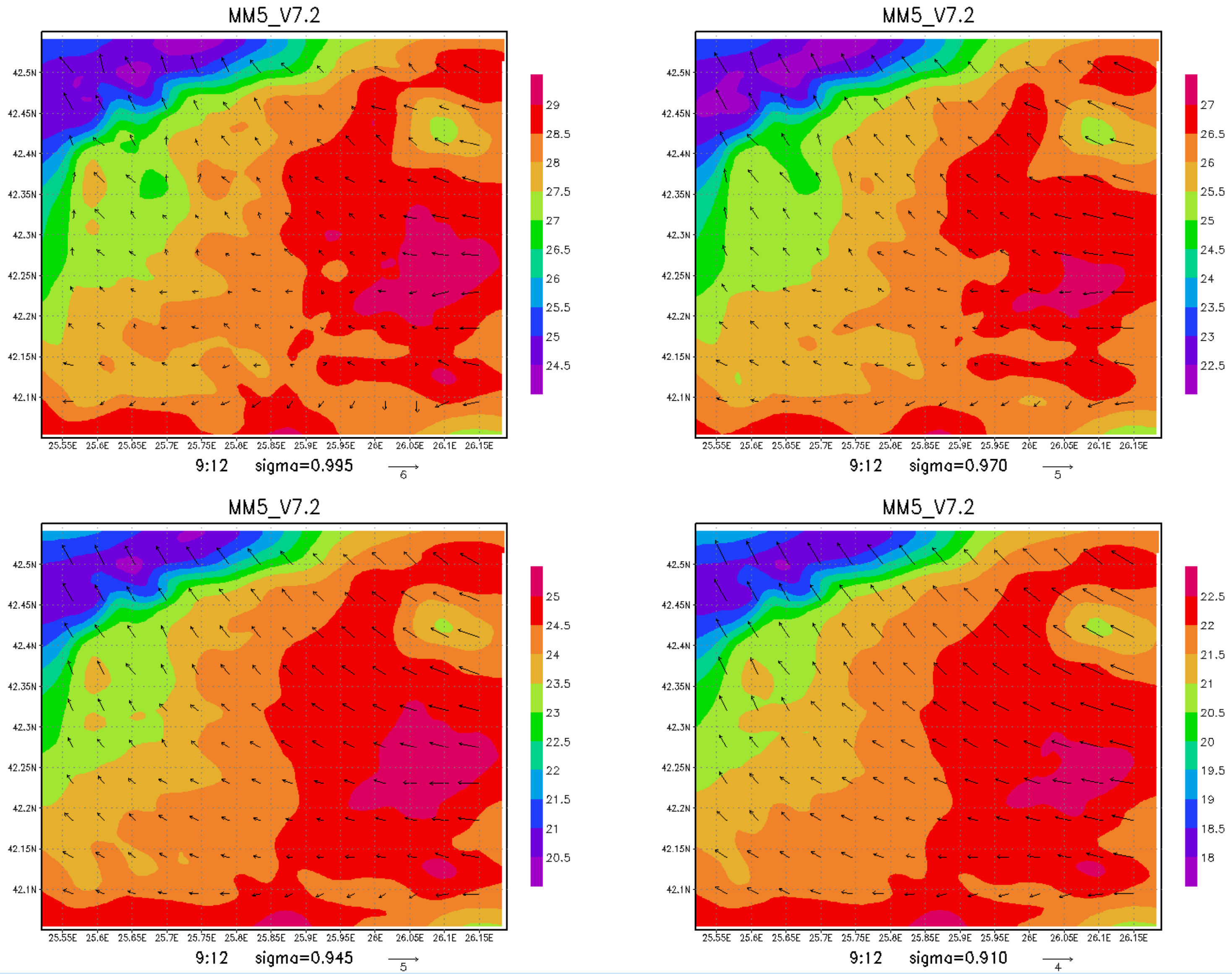


The main impression from the analysis of time and space variation of the wind fields during the period is that calm and non-oriented winds prevail.

There is a very fast change of wind directions in the different points from the region and at different levels.

All this breaks the first hypothetical mechanism able to explain the observed concentration behavior.

7. PREPARATION OF INPUT TO CMAQ

- meteorological

MM5 4.5-days output file	→	CMAQ module MCIP, v.2.3	→	Four met-files for 8, 9, 10 and 11 July 2005 CMAQ met-input

MCIP – Meteorology-Chemistry Interface Processor is performing:

- **Vertical interpolation - from MM5 levels to CMAQ levels**
- **Horizontal adjustment (dot-points ↔ cross-points)**
- **Decrease of CMAQ area with 3.5 points from every side**
- **Preparation of turbulence fields**
- **Preparation of surface fluxes (in accordance with the land-use)**

This procedure was repeated for all domains D1-D5, because MCIP needs information from the rougher domain as to prepare the surface boundary conditions of the next domain in the hierarchy.

CMAQ was run only on the two inner domains with dimensions:

- **3-km resolution domain - 30×30**
- **1 km resolution domain - 48×48**

- emission

Presumption: TPPs are THE ONLY SO_x SOURCE, reasons

Sparse Matrix Operator Kernel Emissions Modeling System - SMOKE, v. 2.0

Purpose of SMOKE - to convert the emission inventory data (annual basis) to the space and time resolution needed by the air quality model through:

space allocation, temporal allocation & chemical speciation

In the case of the “Maritza-Iztok” TPP simulations we have 3 elevated point sources and the SMOKE module ELEVPOINT is activated, fed by the data in the Table above and some ambient air characteristics provided by MM5 simulations.

In this regime SMOKE performs the following operations:

1) Calculates the plume rise - Brigs formuli
2) Calculates the plume vertical spread
3) emission horizontal spatial allocation
4) Transforms emission inventory through temporal allocation (hourly)
5) Creates an CMAQ emission input file in NetCDF format.

- **initial and boundary conditions**

A. Boundary conditions

Following the same presumption, zero boundary conditions are assumed for the outer domain with 3-km resolution. The boundary conditions for inner domain (1-km resolution) are obtained by CMAQ nesting capabilities.

B. Initial conditions

Zero initial conditions are assumed for the first day of simulation (08.07.2005). Initial conditions for the next day are the final pollution fields of the previous day.

Two ways with equal result were exploited for the purpose:

1. CMAQ pre-processors ICON and BCON run with default initial and boundary profiles ? NetCDF files ? conversion to ASCII files ? creation of similar files with zero values ? conversion to NetCDF format.

2. In the CMAQ default concentrations profiles (ASCII files) values replaced with zeros. ICON and BCON run with this modified default profiles.

8. CMAQ SIMULATIONS

CMAQ as well as the others CTMs solves the diffusion equation:

$$\frac{\partial c_i}{\partial t}+\frac{\partial (uc_i)}{\partial x}+\frac{\partial (vc_i)}{\partial y}+\frac{\partial (wc_i)}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial c_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial c_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c_i}{\partial z}\right)+R_i+S_i+D_i+W_i$$

The period 08-11 July 2005 simulated day by day, LINUX scripts created.

Aqueous phase CB-4 chosen for optional chemical mechanism

Many runs were performed !!!

In the first group of runs 6-layer structure of CMAQ is set, levels as follow:

In the second group of runs 14-layer structure of CMAQ is set, levels as follow:

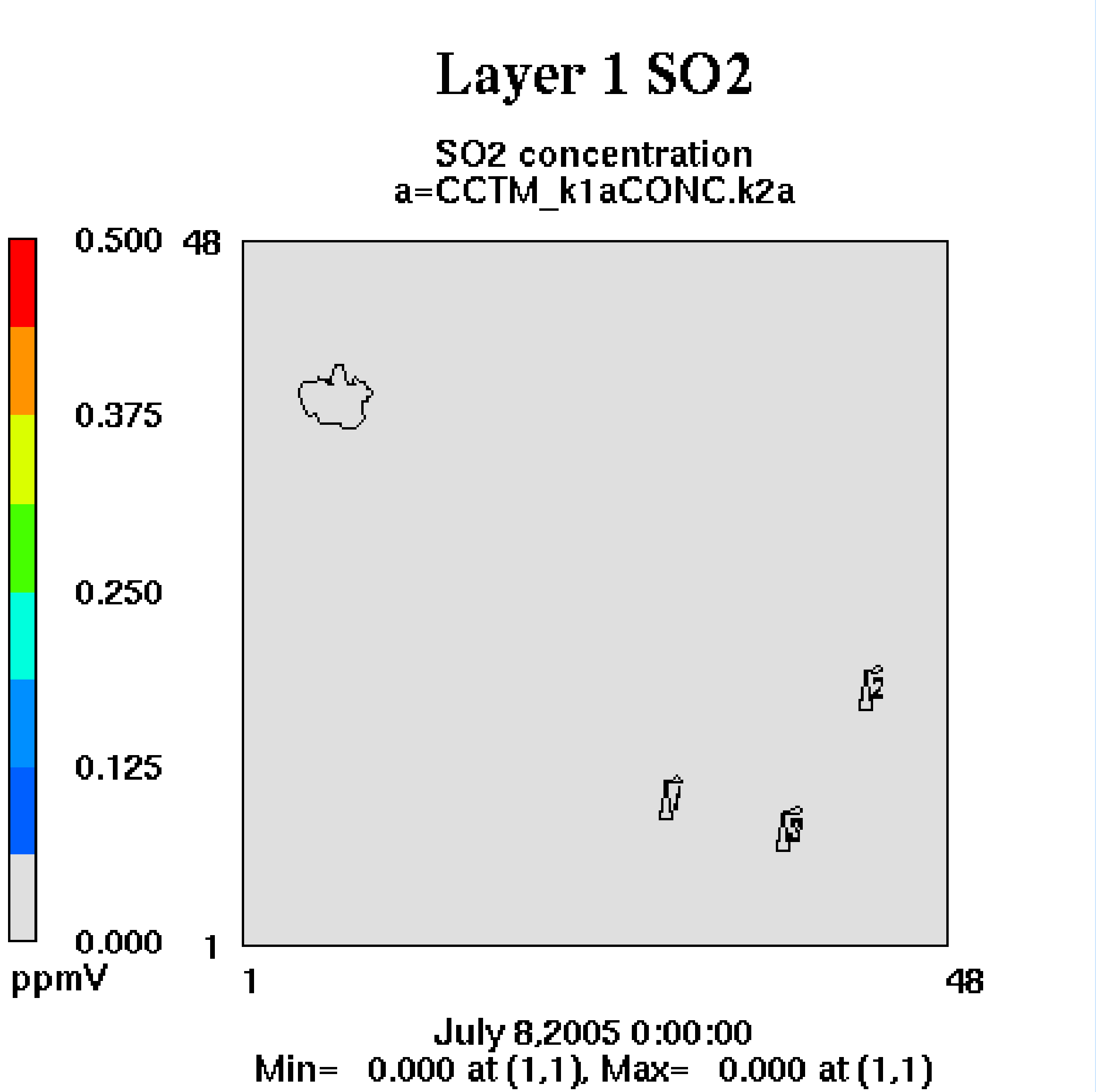
No	1	2	3	4	5	6	7	8	9	10	11	12	13	14
σ	1.0	0.99	0.98	0.96	0.93	0.89	0.84	0.78	0.7	0.6	0.5	0.4	0.3	0.2
h, m	0	76	152	307	554	868	1289	1818	2570	3600	4754	6073	7621	9512

9. DESCRIPTION OF THE EVOLUTION OF THE SURFACE SO_2 CONCENTRATION FIELDS

ONLY 1-km fields discussed here

Animation of the hourly concentration fields:

- **day by day**
- **for all period**


Layer 1 SO2
SO2 concentration
a=CCTM_k1aCONC.k2a
0.500
0.375
0.250
0.125
0.000
ppmV
48
1
1
48
July 8,2005 0:00:00
Min= 0.000 at (1,1), Max= 0.000 at (1,1)

10. ANALYSIS OF THE RESULTS

The presented results show that, in spite of numerous runs with different parameters, the calculated concentrations in the points with measurements do not follow the observations.

It must be mentioned, however, that every day, in the afternoon, pollution spots near Stara Zagora can be observed, but they almost do not cover it.

Reasonable behavior of calculated field from physical point of view:

- **In night hours, in relatively stable PBL, the pollution released from elevated sources keeps aloft**
- **In day hours the fast development of turbulent mixing drains the pollution to the surface (plumes formed)**
- **Only in the night of 10-11 July 2005 a surface pollution spot of about 100 ppb is observed at the NW domain edge, beyond Stara Zagora**

This is quite reasonable for summer time and is discussed by many authors (Palau et al., 2005, Hurley and Physick, 1991, Luhar, 2002, Luhar and Young, 2002, and others).

All this show that the second physical hypothesis discussed in § 2 (Description of the pollution episode) is possibly in force:

- Suitable direction of the wind from TPPs to the town of Stara Zagora is observed in the afternoons each one of the days;
- Pollution spots in different places around the town are formed, but not over.
- Deviation of the wind direction with some degree or change of the wind speed with some m/s can form spot over the town in the right periods.
- Small changes in the PBL height and turbulent mixing can lead to similar results.

All difficulties trying to model local scale phenomena in complex condition reveal!

<u>Our opinion:</u> **the main shortcomings come from the MM5 simulations**

Several reasons for false simulation can be identified:

- weak winds – uncertain PBL parameterization – local inhomogeneities
- unstable wind direction – insufficient adaptation time
- insufficient vertical resolution of the model

All this means that in the case of tall stacks and considerable initial plume rise, the meteorological conditions at upper levels are critical for the plume spread.

11. CONCLUSION, PLANS FOR FURTHER EXPERIMENTS

In general, we conclude that the presented modeling results are reasonable. At this stage, the observed SO_2 episodes in summer 2005 cannot be explained quantitatively. Validation data for the meteorological model are necessary.

This results can convince the government in the necessity of organization of experimental studies that can help the air quality management in the region of Stara Zagora.

In a state of no validation data, numerical experiments can continue by:

- Increase of the number of vertical levels, better resolution in PBL;
- Different PBL parameterization schemes must used;
- Make use of other input meteorological data sets – ECMWF, ALADIN, HRM;
- Additional emission scenarios applied (as in Palau et al (2005).

ACKNOWLEDGEMENTS

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