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High-resolution pollutant dispersion modelling in contaminated coastal sites

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Abstract

The recent developments in pollutant measurement methods and techniques necessitate improvements in modelling approaches. The models used so far have been based on seasonally averaged data, which is insufficient for making short-term predictions.

We have improved the existing modelling tools for pollutant transport and dispersion on three levels. We significantly refined the numerical grid; we used temporally and spatially non-uniform meteorological parameters for predicting pollutant dispersion and transformation processes; we used grid nesting in order to improve the open boundary condition. We worked on a typical contaminated site (The Gulf of Trieste), where mercury poses a significant environmental threat and where an oil-spill is a realistic possibility. By calculating evasion we improved the mass balance of mercury in the Gulf. We demonstrated that the spreading of river plumes under typical wind conditions is different than has so far been indicated by model simulations. We also simulated an oil-spill in real time.

The improved modelling approaches and the upgraded models are now suitable for use with the state-of-the-art measurements technology and can represent an important contribution to the decision-making process.

Keywords: mathematical modelling, hydrodynamic circulation, Gulf of Trieste, pollutant dispersion, mercury, evasion, oil-spill

1. Introduction

The presence of various pollutants in marine contaminated sites is a growing global concern. Monitoring their levels, transformations and dispersion is therefore crucial. In the last decade measurement methods and techniques have been significantly improved. Within the EU FP7 project “Hydronet” (http://www.hydronet-project.eu/), a new automatized measurement system was developed to improve the efficiency of pollutant monitoring in contaminated sites. Similar autonomous systems are also being developed elsewhere, e.g. by the NOAA (http://www.nauticalcharts.noaa.gov/csdl/AUV.html) and Harpha Sea (http://www.harphasea.com/index.php/en/products/automatic-vessel). Particularly in small areas, automatized systems can harvest data in high spatial and temporal resolutions, and enable tracking of extreme and unexpected events. This provides an excellent early warning system for detecting increased risk of pollution in wider geographic areas. Furthermore, new methods for continuous measurements of pollutant distribution and concentrations in water have also become available (Andersson et al., 2008; Gårdfeldt et al., 2003), providing more complete time series of data. The considerable technological improvements in data acquisition subsequently require improved modelling tools.

Several new approaches in modelling are currently being developed. Machine learning tools can efficiently use the spatial and temporal high frequency measurements for predicting contaminant distribution and particularly transformation processes. Their main drawbacks are the need for complete time-series of measurements, which are difficult to obtain, and the lesser transparency of such models (Žagar et al., 2007). Another modelling approach involves simulations of pollutant transport, dispersion and transformations based on hydrodynamic modelling. Such an approach enables more exact simulations of contaminant spatial distribution. Moreover, changing the model parameters is relatively easy and thus future scenarios can be simulated.

Increasing processor abilities have enabled significant refinement of numerical grids. A decade ago, the grid resolution in a typical contaminated site (e.g. the Gulf of Trieste, area approx. 600 km^2) was in the order of magnitude of 500 m and the number of computational elements did not exceed 50,000 (Rajar et al., 2000). Recently, 150 m resolution with well over a million computational elements was used in the same area (Žagar and Ramšak, 2010). In certain sub-areas of the Gulf of Trieste, such as the Koper Bay, it has even been refined further to approx. 40 m (Žagar et al., 2012).

Modelling in contaminated sites has traditionally been performed with annually or, in the best case, seasonally averaged input data (Horvat et al., 1999; Rajar and Četina, 1997; Rajar et al., 1997; Rajar et al., 2000; Širca et al., 1999b). Real-time data was mostly unavailable and has only been used for calibration and validation of models. Even in such case studies, forcing factors were spatially averaged in smaller domains not exceeding a few hundred square kilometres, which are the usual dimensions of contaminated sites (Rajar et al., 2004; Žagar, 1999; Žagar et al., 2001). While appropriate for predicting long-term pollutant dynamics and establishing annual mass balances (Rajar et al., 2007; Rajar et al., 2004; Širca et al., 1999a), using averaged input data cannot accurately describe the dynamics of short-term processes. Transport, fluxes and transformations in contaminated areas are highly susceptible to hourly changes in meteorological conditions and a wide range of other environmental parameters that also change with high frequency.

With the development of nearly real-time simulations in contaminated sites, the need for quality input data on hydrodynamic circulation, meteorological situation and physico-chemical parameters has also increased drastically. Adequate data are available from various databases and forecasting systems, which are in many cases products or parts of on-going research projects. Large databases of measurements and modelling results are available on-line (e.g. the Mercyms project http://www.ist-world.org/ProjectDetails.aspx?ProjectId=3caaba5b92474b60a544327b8e2e821a, MODB http://modb.oce.ulg.ac.be/). For the wider Mediterranean area meteorological forecasts in high spatial and temporal resolution (hourly on 1/20 deg) are available on request from the University of Athens (http://forecast.uoa.gr/), while regional Environmental Agencies (e.g. the Slovenian Environment Agency, http://meteo.arso.gov.si/met/en/) produce meteorological forecasts in even finer spatial scale of a few kilometres. Freely available products of the EU FP7 project MyOcean (www.myocean.eu/) contain 10-day forecasts and reanalyses of ocean circulation on a daily temporal scale with spatial resolution of 1/16 degree for the entire Mediterranean Sea. Satellite observations and cruise measurements are also available for the Mediterranean and several other seas and oceans. In the framework of the same project, chlorophyll, oxygen and nutrient concentration forecasts in the surface layer and in the water column are available, as well as reanalyses of the same data.

Using all these data as input for refined high-resolution simulations in contaminated sites in combination with advanced modelling techniques undoubtedly represent a much better support to the advances in measurement techniques. In this way the modelling results (on hydrodynamics, transport and dispersion, and transformations) can be used for planning sampling campaigns and for source finding, and thus for increasing the efficiency of measurements. On the other hand, high resolution and high frequency sampling data on contaminants and water quality parameters enable better calibration and validation of models and as such increase their reliability.

We present the gradual improvement of the three-dimensional models PCFLOW3D and Nafta3D in the last few years. Three case studies are shown that demonstrate the advancement in grid refinement and different approaches in data averaging. Simulations with temporal and spatial high resolution data in the Gulf of Trieste are shown. The upgraded model is ready to support automatized measurements of pollutants in contaminated sites and has been successfully applied in the framework of the EU FP7 project “Hydronet”.

2. *Methods*

2.1 Description of the models

The PCFLOW3D is a non-steady state three dimensional non-linear baroclinic z-coordinate numerical model with a hydrostatic approximation. The model was developed at the Faculty of Civil and Geodetic Engineering of the University of Ljubljana and consists of four modules: a hydrodynamic (HD) module, a transport–dispersion (TD) module, a sediment-transport (ST) module and a biogeochemical (BGC) module with the ability to simulate basic mercury transformations in the water column and fluxes between the environmental compartments. The wind-induced, tidal and thermohaline forcing as well as inflow momentum of rivers can be taken into account as forcing factors. Smagorinsky and Mellor-Yamada turbulence models were used in the horizontal and vertical directions, respectively. The transport equation in the model can be solved either by an Eulerian finite difference method (FDM) or a Lagrangean particle tracking method (PTM). FDM was used for simulations of dissolved pollutants and PTM for oil-spill simulations. The ST module is similar to the model of Lin and Falconer (1996), and solves the advection dispersion equation where the empirical equation for the sedimentation velocity of non-cohesive sediment is accounted for (van Rijn, 1993). The sedimentation and resuspension of sediments from the bottom are calculated as a result of the shear stress produced by the combined impact of currents and waves. Wind-induced waves are approximated as proposed by Brettschneider (1952). The BGC module of the PCFLOW3D model accounts for three mercury species: gaseous elemental mercury (Hg^0); and divalent (Hg^{2+}) and mono-methyl (MMHg) mercury in dissolved and particulate forms. The basic mercury transformation processes (methylation, demethylation, reduction and oxidation) are simulated using spatially and temporally variable transformation coefficients in each cell of the three-dimensional computational domain. The module takes into account exchange with the bottom sediment (diffusive fluxes from sediment to the bottom layer) and exchange with the atmosphere (evasion from the surface layer as well as wet and dry deposition).

A detailed description of the individual modules and the PCFLOW3D model is given in Rajar et al. (1997), Četina et al. (2000), Rajar et al. (2004) and Žagar et al. (2007). The model has been applied for many practical problems of pollutant dispersion (Četina et al., 2000; Malačič et al., 2010; Rajar et al., 1997; Rajar and Širca, 1996, 1998) with the main focus on mercury transport and transformation processes in the Gulf of Trieste (Rajar et al., 2000), Minamata Bay (Rajar et al., 2004) and the entire Mediterranean (Žagar et al., 2007).

The Nafta3D is a three-dimensional Lagrangean model for oil-spill simulations. The advection fields from the PCFLOW3D hydrodynamic module, the Princeton Ocean Model (POM, http://www.aos.princeton.edu/WWWPUBLIC/htdocs.pom/) for the Gulf of Trieste and the Northern Adriatic, or any other structured grid hydrodynamic model can be transformed into input data for oil-spill simulations using adequate interfaces. Velocity fields are further interpolated in time and space in order to exactly determine the velocity and displacement of individual particles. Dispersion is modelled by statistically appropriate random-generated values within the limits of the horizontal and vertical turbulent diffusion coefficients. Furthermore, buoyancy of oil is accounted for in the vertical direction. The Nafta3D model computes several processes of oil transport and fate: advection and dispersion, mechanical spreading, evaporation, emulsification and dispersion in the water column. The model and the basic equations of the included processes are described in Delgado et al. (2006) and Žagar et al. (2011).

2.2 Case studies

Three case studies in the Gulf of Trieste (Figure 1) are presented: in the first, high resolution temporal data were used to determine mercury evasion. The second shows the use of spatial high resolution data in order to refine simulations of dissolved pollutants in the vicinity of the Soča/Isonzo river mouth. In the third case study we used temporal and spatial high resolution data for simulating oil-spills.

2.2.1 Case-study A: Modelling mercury evasion in the Gulf of Trieste

Širca et al. (1999a) established the annual mercury mass balance of the Gulf of Trieste based on annually averaged input data, which were adequate for the computation of river inputs, basic mercury transformations and fluxes between the water and bottom sediment. Mercury evasion from the Gulf was not calculated but rather estimated to the order of magnitude. As shown in several experimental and modelling studies (Andersson et al., 2007; Andersson et al., 2011; Gårdfeldt et al., 2003; Žagar et al., 2007), the evasion of mercury as well as other volatile pollutants is highly dependent on the wind and several other parameters such as temperature, sun light, availability of Hg^{2+} for reduction, etc. The dependence on wind is non-linear and can be parameterised by different equations (Nightingale et al., 2000; Wanninkhof, 1992; Wanninkhof and McGillis, 1999). In order to accurately predict the evasion, averaging of wind over longer periods is not adequate. Due to relatively complicated topography of the mainland, only the Beli Križ station was found to be representative of wind measurements. The year 1988 was chosen as representative for the simulations (Širca et al., 1999a; Širca et al., 1999b). Measurements were available for the entire year and the seasonally averaged wind data was used for hydrodynamic simulations (Rajar et al., 2000; Žagar et al., 2001). Hourly wind speed and direction data were used to calculate evasion.

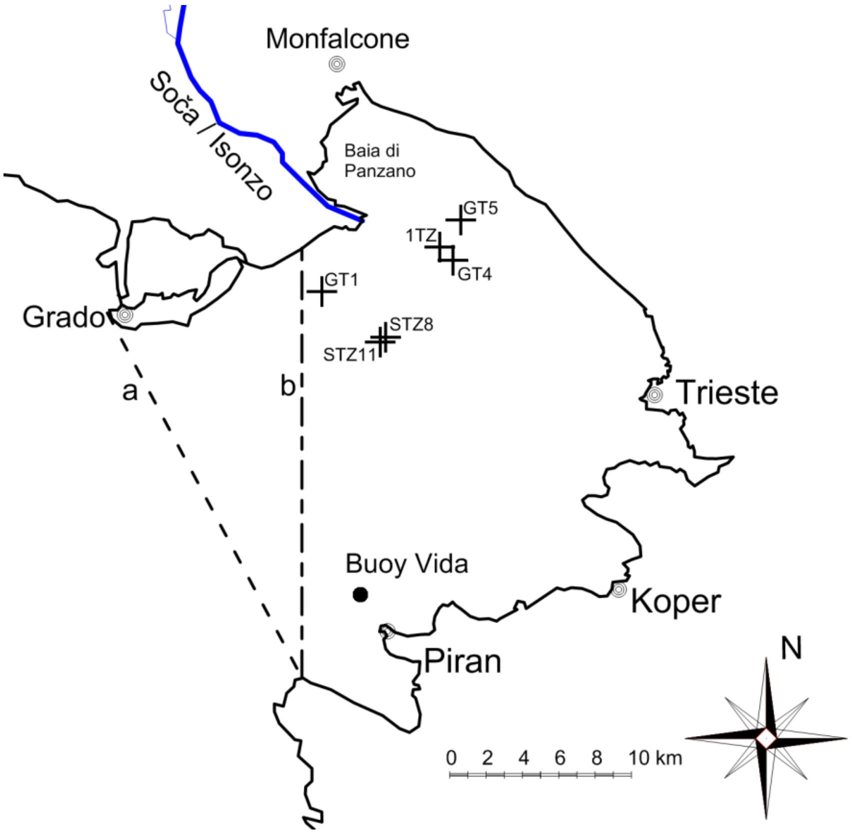

Figure 1: The Gulf of Trieste with the location of the buoy, sampling locations and the open boundary in the first case study (a) and the other two studies (b).

In the water compartment, seasonal circulation and the distribution of temperature and salinity were calculated for each season and for two additional inserts of high river discharge, as described in Žagar et al. (2001). The numerical grid with a spatially non-uniform horizontal resolution between 300 m at the Soča/Isonzo river mouth, and 900 m at the open boundary was applied. In the vertical direction the computational domain was divided into 25 one-meter thick layers. Transport, dispersion and transformations of three mercury species were simulated. The reaction coefficients proposed by Širca et al. (1999b) were corrected as described in Žagar et al. (2007) in order to take into account the seasonal variability and the variability along the water column. Mercury deposition was determined by seasonal simulations using the Rams-Hg model (Kallos et al., 2001) in the framework of the Mercyms project (Žagar et al., 2007). Total gaseous mercury (TGM) in the air above the Gulf was measured according to the method described in Andersson et al. (2007). Seasonally measured concentrations of mercury species were available for calibration of the model in the water compartment. Dissolved gaseous Hg (DGM) and reactive Hg (RHg) were determined on board the sampling vessel. Immediately after sampling the sample for DGM was transferred into a glass bubbler. It was purged for 10 min and collected on a gold trap which was then transferred to a double amalgamation cold vapour atomic absorption (CV AFS) analyser system. Hg on the sampling gold trap was then released by thermal desorption and detected by a CV AFS analyzer (Tekran 2500). The method is described in detail in Horvat et al. (2003) and Gardfeldt et al. (2003). It should be noted that DGM concentrations reported in this study correspond to all volatile Hg species present in sea water – elemental Hg (Hg^0) and dimethyl Hg ($(CH_3)_2Hg$). For RHg determination an aliquot of the sample was transferred directly from the Niskin sampling bottle to a reduction vessel containing $SnCl_2$ solution in H_2SO_4 to reduce free inorganic Hg^{2+} to Hg^0. Reduced Hg^0 was amalgamated on a gold trap followed by thermal desorption and detection by Milton Roy cold vapour atomic absorption spectrometer (CVAAS). The results provided in the tables and figures were corrected for DGM and represent reactive Hg (Hg^{2+}) calculated from the difference between DGM and measured "reactive Hg". A detailed description of the method is given in Horvat et al. (Horvat et al., 1991; Horvat et al., 1987)).

Evasion was calculated using the Wanninkhof's parameterisation (Wanninkhof, 1992), as described in Gårdfeldt et al. (2003) and Žagar et al. (2007) with hourly winds. Preliminary computations showed that evasion significantly exceeded deposition and river inflow of dissolved mercury. Therefore, additional mercury fluxes from sediment were taken into account, as quantified in Širca et al. (1999a) and Covelli et al. (1999), in order to keep seasonal mercury concentrations in the water column in accordance with measurements.

The evasion values computed by the PCFLOW3D model were verified by a calculation in the Excel 2003 for Windows, where the hourly wind data within each season were sorted in classes with the interval 1 m s^{-1}. The number of hours within each interval was determined and evasion was calculated for each interval as described in Gårdfeldt et al. (2003).

2.2.2 Case study B: Dispersion of pollutants in the vicinity of the Soča/Isonzo river mouth

Large quantities of particulate and dissolved mercury are being carried into the Gulf of Trieste more or less regularly by the rainfall and snowmelt-induced flood waves (Širca et al., 1999b; Žagar et al., 2006). Furthermore, the concentrations in the bottom sediment of the Gulf reach up to 50 ppm (Covelli et al., 2001). Some of the mercury-rich sediment is being resuspended and carried away from the Soča river mouth, particularly in winter months, when strong wind (bora) induces stronger currents and high waves (Rajar et al., 2000; Žagar, 1999). All previous mercury modelling studies in this area were performed on hydrodynamic simulations with spatially homogeneous wind over the basin. Moreover, in such small areas this is the usual approach in hydrodynamic modelling studies (Crise et al., 2006; Malačič and Petelin, 2009).

In this case study, two typical wind forecasts of the Slovenian Environment Agency with spatial resolution 2.5 km were used as input data. The bora-wind forecast for 25 Feb 2009 was used (average strength 6.95 m s^{-1} and direction 66.6°), and for scirocco, the forecast was for 3 Mar 2009 (average velocity 1.76 m s^{-1} and direction 255.9°). Wind fields were interpolated to the numerical grid of the PCFLOW3D model (approx.150 m resolution) using cubic polynomial interpolation. Well mixed winter conditions with temperature 8.5° and salinity 36 psu were used. The circulation in the Gulf was determined using both uniform and non-uniform wind fields, which were kept constant in time. The simulation time was 24 and 36 hours for the bora and scirocco winds, respectively, in order to reach stationary circulation. The results of the hydrodynamic simulations were validated on measured velocities at the buoy 'Vida' close to the Slovenian coast in front of Piran (http://buoy.mbss.org/).

Using stationary velocity fields from the PCFLOW3D hydrodynamic module, twelve-hour simulations of dissolved passive pollutant were performed for the four wind cases. The average discharge of the Soča/Isonzo (150 $m^3\ s^{-1}$ at the river mouth) was used; the initial concentration in freshwater was set to 100.

2.2.3 Case study C: Simulation of an oil-spill during a short-term real-wind event

Two ports with oil-terminal facilities are situated in the southern part of the Gulf of Trieste. Tanker traffic with crude oil and derivatives in the area is relatively high: 405 tankers navigated to the Port of Trieste and 220 to the Port of Koper in 2005 (MOP, 2008). A larger oil-spill in this area has not yet been recorded. In case of an oil-spill event, it is very important to begin remediation measures immediately, before the slick is too large to control. At this stage, accurate prediction of slick propagation and dispersion is crucial, while the significance of other processes (evaporation, emulsification, biodegradation etc.) increases in later stages of the spill, when the environmental impact and fate of the spilled oil are being determined. Mathematical models of oil propagation and fate are a valuable tool that is often used in both stages.

In this study the hydrodynamic circulation computed with the TSPOM model based on spatially and temporally variable wind was used (Malačič et al., 2010). A three-day wind forecast of the Slovenian Environment Agency for the period between 19 and 21 Mar 2009, when two wind overturns occurred (scirocco – bora – scirocco), was interpolated to the numerical grid of the hydrodynamic model. In the TSPOM computations the numerical grid resolution was approx. 150 m in the horizontal plane with 11 σ-layers down the water column. The open boundary condition was obtained from one-way nesting of the computational domain into the NAPOM (North Adriatic POM model domain).

NAPOM (Malačič et al., 2012) is an operational variant of the Princeton Ocean Model covering the northern part of the Adriatic sea. The domain boundaries are 44.478°N - 45.82°N and 12.20°E - 13.91°E, and its rectangular horizontal grid has a typical horizontal resolution of roughly 600 m with 11 σ vertical layers reaching maximum depth of 53 m. The model is initialised and forced by the Adriatic Sea Forecasting System (run by INGV Bologna http://gnoo.bo.ingv.it/afs). TSPOM is a variant of the Princeton Ocean Model covering the Gulf of Trieste, initialized and forced by the NAPOM operational model outputs, which are spatially and temporally interpolated to the TSPOM grid and time-step requirements. Both models use two time step modes for computation: the external time step for barotropic-mode computation, which is explicit in time and covers fast-travelling signals (surface elevation and long waves); and the internal time step used in implicit-mode computation. The time steps in both models satisfy the Courant-Friedrich-Levy condition for numerical stability. The internal time steps for the NAPOM and TSPOM models are 90 and 30 s, respectively, and the external time steps are 9 and 2.5 s, respectively.

As both models use the same vertical resolution (11 σ -layers), the adaptation of NAPOM results is only performed in the horizontal direction. The relatively large difference in horizontal numerical resolutions between TSPOM and NAPOM grids arises from the fact that we cannot afford time-consuming multi-level nesting in the current operational chain due to the time constraints imposed by the Administration for Civil Response and Disaster Relief.

Beside wind and the open boundary condition, climatological discharges of rivers Soča/Isonzo, Dragonja, Rižana and Badaševica were taken into account as boundary conditions.

Hourly three-dimensional velocity fields of the TSPOM model were transformed into the input data for the Nafta3D model and used for oil-spill simulations. In the horizontal plane the numerical grid of the Nafta3D model is of the same resolution as in the previous case-study and in the TSPOM model. In the vertical direction in the Nafta3D model, the computational domain is divided into 13 *z*-layers of different thicknesses, from 30 cm at the surface to 5 m at the bottom. Therefore, velocities had to be transformed from σ to *z* coordinates in each grid cell. Velocity fields are further interpolated in space and time to the exact locations of individual oil particles.

A potential oil-spill in the vicinity of the Port in Koper was simulated with and without evaporation. Diesel-fuel spill was modelled, where evaporation of light oil fractions is considerable. A typical diesel fuel with characteristics as described in Mackay et al. (1980) and Fingas (2011) was used in the simulations (Table 3). Both simulations were performed with a 500 ton spill in 5 hours at the same location (φ = 45.55°, λ = 13.7°) and 10,000 particles were used in each case. Water temperature was set to 10°C. The simulation time was 70 hours with a 6 minute time step. In each cell of the numerical grid concentrations of oil were computed from the (remaining) mass of the oil particles.

3. *Results and discussion*

3.1 Case study A: Mercury evasion in the Gulf of Trieste

Seasonally averaged parameters used in the Excel computations according to Gårdfeldt et al. (2003) are given in Tables 1 and 2 for the water and the air compartment, respectively. In computations with the PCFLOW3D model only the atmospheric (deposition and TGM) data and the bottom fluxes were kept constant throughout the season, while all other parameters were calculated for each grid cell in every time step (5 minutes). The total annual deposition calculated with the values from Table 1 (approx. 9.5 kg) is in relatively good agreement with the 5.5 kg of annual wet deposition suggested in Širca et al. (1999a). The annual dissolved mercury flux from the sediment was calculated to be approx. 23 kg, which is about 5% of the total flux suggested in Širca et al. (1999b) and Covelli et al. (1999). The reason for this discrepancy is that the bottom fluxes suggested in Širca et al. (1999b) and Covelli et al. (1999) were determined for total (dissolved and particulate) mercury. However, only a small fraction of mercury is in dissolved form and thus directly capable of transformations and evasion. The model was calibrated with the measured dissolved Hg values and the estimated bottom fluxes (Table 1) were taken into account in the final simulations.

The model was validated with DGM measurements in the water column performed in late spring (25 Jun 2005), late summer (23 Sep 2003) and late autumn (2 Nov 2004). The agreement along the water column was within a factor of two and in most cases significantly better at the surface (Figure 2). Some discrepancies in lower layers were observed. The transformation coefficients used in the model probably do not accurately describe all the biotic and abiotic Hg transformation processes taking place in the water column.

The agreement of evasion calculated with the PCFLOW3D model and with the method of Gårdfeldt et al. (2003) is also within the factor of two (Table 2). Considering the averaging of parameters in the Excel calculations the lower quantity obtained with the PCFLOW3D model was expected. A similar discrepancy between modelling results and manual calculation from measured data (approx. 40%) was also noticed in the Mediterranean Sea (Andersson et al., 2007; Žagar et al., 2007). One of the possible reasons is that the modelled DGM concentrations in the surface layer vary significantly due to transformations and evasion, which is not accounted for in manual calculations. Furthermore, the real wind sequels used in the modelling simulations show much higher variability in time than either the representation with wind classes used in the Excel calculations or averaging of wind over longer periods. The sensitivity analysis of the chosen gas exchange model showed high correlation of wind and DGM with evasion, while correlations with all other parameters were lower (Žagar et al., 2007).

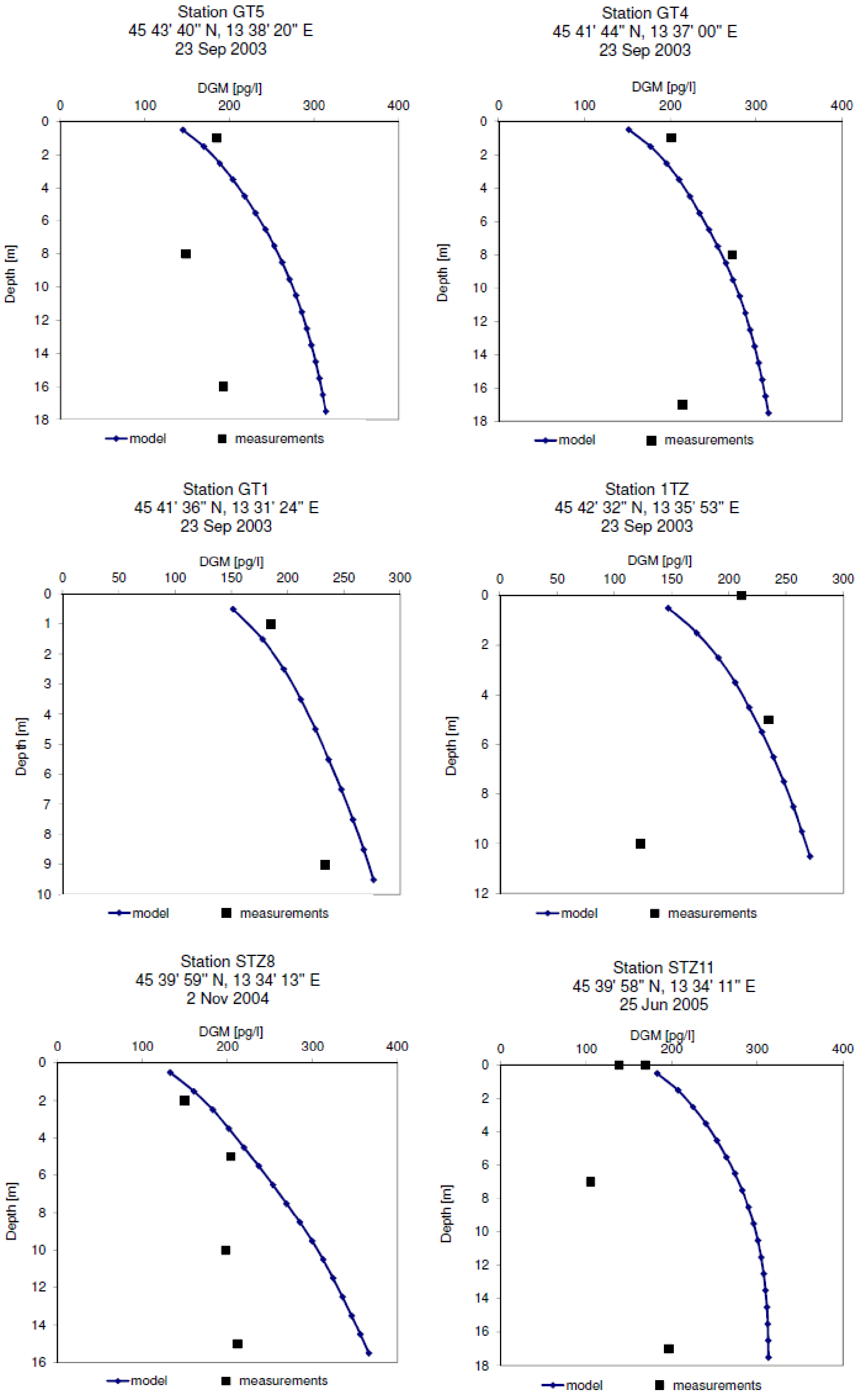

Figure 2: Measured and simulated DGM profiles.

In order to close the mass balance with the higher quantity, additional DGM sources, most likely stemming from the bottom sediment, need to be considered.

Table 1

Seasonal mercury evasion parameters in the water compartment (Sc = Schmidt number, H' = Henry's constant)

Season	T (surface) [°C]	Sc [-]	H' [-]	DGM [pg l^{-1}]	Bottom flux [ng m^{-2} day^{-1}]
Spring	15.8	493	0.2511	153.5	100
Summer	25.1	312	0.3180	246.4	90
Autumn	15.9	491	0.2517	150.0	90
Winter	7.8	761	0.2022	151.8	90

Table 2

Seasonal mercury evasion parameters in the air compartment and calculated evasion

Season	TGM [ng m^{-3}]	Deposition [ng m^{-2} day^{-1}]	Evasion (Gårdfeldt et al. 2003) [kg]	Evasion (PCFLOW3D) [kg]
Spring	2.12	61.2	24.43	17.46
Summer	1.96	28.3	53.65	20.08
Autumn	2.14	70.4	30.39	20.88
Winter	1.92	10.4	24.90	19.47
Annual			133.37	77.89

Širca et al. (1999a; 1999b) assumed volatilisation/evasion to be negligible in comparison with other transport and transformation processes within the Gulf of Trieste. However, the newly computed evasion (approx. 100 kg yr^{-1}) is of the same order of magnitude as the net exchange with the Northern Adriatic and at least by an order of magnitude higher than the deposition and inflow of dissolved mercury with the Soča/Isonzo. Relative to other mercury losses in the system, the evasion term in the Gulf of Trieste is not as important compared to the entire Mediterranean Sea (Andersson et al., 2007; Rajar et al., 2007). Nonetheless, fluxes across the marine boundary layer are a significant sink of dissolved mercury in contaminated sites and should be determined properly.

3.2 Case study B: Pollutant transport near the Soča/Isonzo river mouth

In order to refine simulations of dissolved pollutants in the vicinity of the Soča/Isonzo river mouth, the first step was to determine the hydrodynamic circulation in the Gulf of Trieste, using both uniform and non-uniform wind fields. In the surface layer, the current velocities near the Soča/Isonzo river mouth computed with non-uniform wind were significantly lower than with averaged wind (Figure 3). The modelling results were validated with measurements at the buoy Vida near Piran, Slovenia. For the bora-wind event, the agreement of the results obtained with non-uniform wind was significantly better in both absolute value and direction, while the scirocco simulations showed only slight improvement in comparison to simulations with spatially uniform wind (Figure 4). One of the main reasons is the vicinity of the open boundary. During the scirocco wind event, the impact of currents from the Northern Adriatic (inflow) is more evident than in bora wind conditions (outflow).

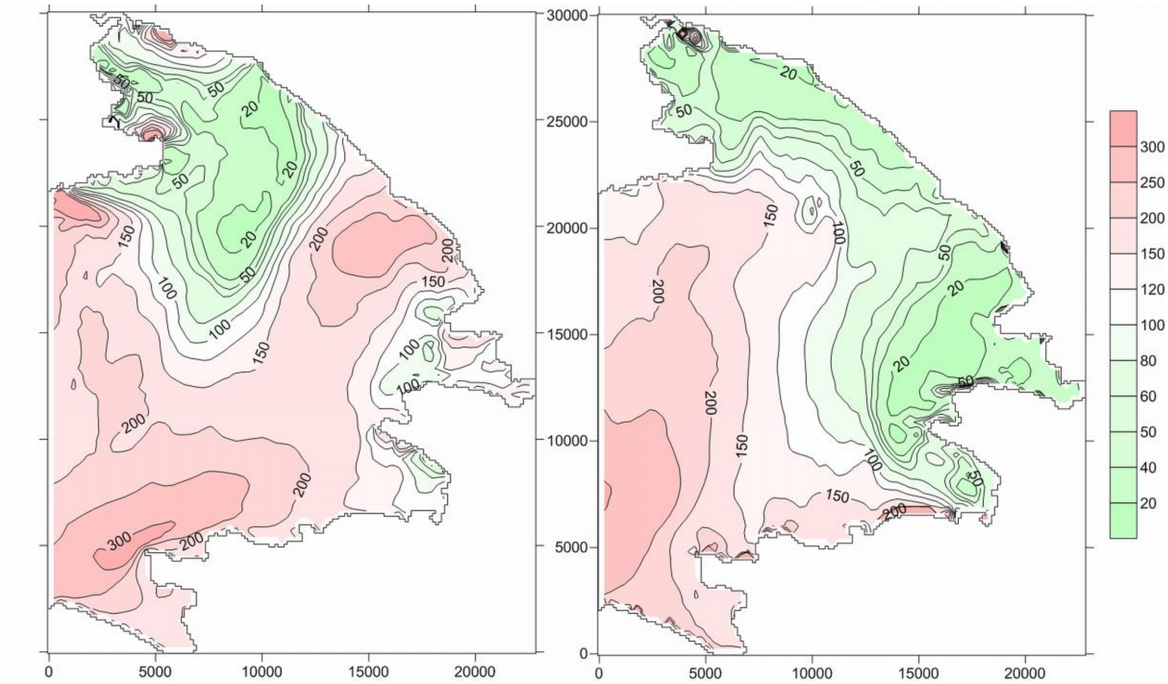

Figure 3: Relative differences (%) in current velocities simulated with spatially homogeneous and non-homogeneous winds in the surface layer; bora (left) and scirocco (right).

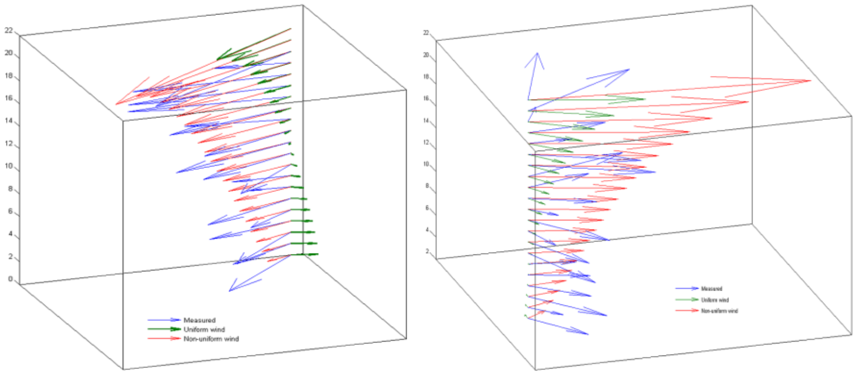

Figure 4: Comparison of flow velocities along the water column at the location of the buoy for bora wind (left) and scirocco (right).

Even after very short simulations of pollutant transport (12 h in each of the four wind cases) the difference in concentrations in the surface layers is evident, particularly in the bora wind event (Figure 5). Previous modelling studies performed in the Gulf of Trieste (Rajar et al., 2000; Širca et al., 1999b; Žagar et al., 2001) resulted in patterns of dissolved and particulate pollutant transport similar to the ones obtained with the spatially uniform wind. Transport into the northernmost part of the Gulf (Baia di Panzano), which is evident from measurements during a similar event (Covelli et al., 2007), was never demonstrated. Instead, the river plume was carried along the north-western coast into the Northern Adriatic. The impact of the Soča/Isonzo river plume on contamination of the Baia di Panzano is, however, much greater: heavy rainfall events in the Soča/Isonzo catchment are usually followed by few-day periods of stronger bora wind. The increased river discharge during such events carries large quantities of pollutants which are dispersed throughout the Gulf in a different pattern than shown by previous modelling simulations.

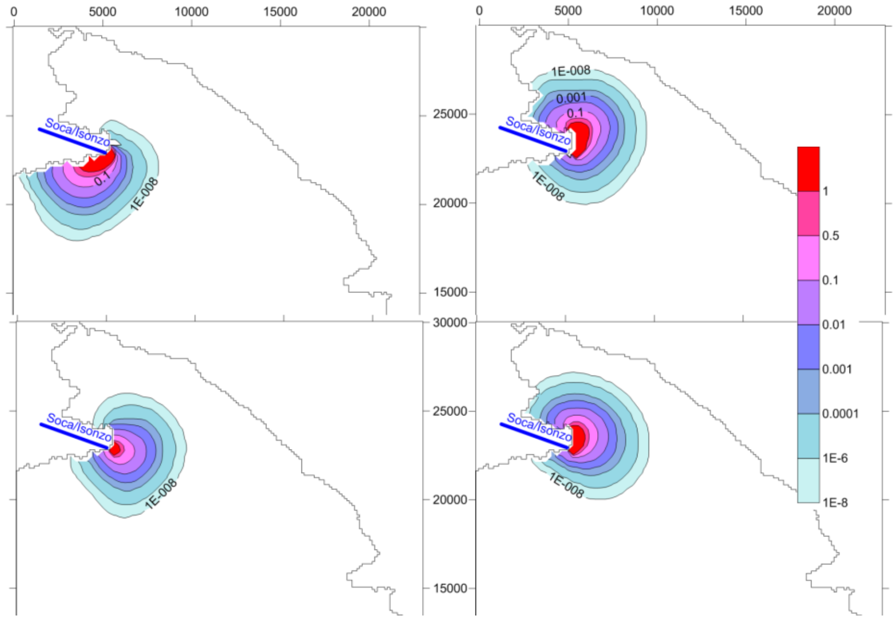

Figure 5: Passive pollutant concentrations in the vicinity of the Isonzo/Soča river mouth after 12-hour simulations. Bora wind (left) and scirocco (right), spatially averaged (top) and non-uniform wind (bottom).

The main concern with mercury pollution in the Gulf of Trieste is high mercury methylation and the risk of elevated methyl-mercury in the marine food chain. Due to fish farming and mariculture in the area of Baia di Panzano this part of the Gulf is particularly susceptible to changes in mercury levels and exhibits a relatively high Hg methylation potential (Hines et al., 2006). The modelling approach with spatially variable wind has indicated that during regular flood events, the area of Baia di Panzano is under higher risk of Hg pollution than was previously thought. Therefore, future modelling simulations should be performed with circulation based on spatially non-uniform wind. Otherwise, it is not possible to adequately demonstrate the important short-term pollutant transport and transformation processes, and quantify present and future levels of pollution.

3.3 Case study C: Oil spill during a short-term real-wind event

Oil spills can be modelled in two ways: the tactical modelling approach is applied after occurrence of a spill and the results need to be made available in the shortest possible time; while the prognostic (forecasting, hindcasting) modelling is used to predict or analyse the environmental impact or possible scenarios of oil propagation and fate. In the first case, all long-term processes and even evaporation are often excluded from simulations in order to shorten the computation time. Three-day simulations were performed with and without evaporation and both took less than an hour on a single Intel Core i7 processor. The difference in computational time was less than 10%. As tactical modelling is usually performed only for a period of a few hours, the results are available in a few minutes. Although slightly slower, the simulations with evaporation provide more exact information on the quantity of the remaining oil and on adequate mitigation measures.

The quantities of remaining oil simulated with and without evaporation for different times after the spill are given in Table 4. It is evident that after only 5 h, when the spill ceased, almost half of the diesel-fuel had evaporated. In this time the slick covered an area of 2.6 km^2, which is due to low viscosity of the selected fuel and the relatively high wind speed. In such cases it is crucial that remediation begin as soon as possible. After only a few hours, the size of the slick makes it exceedingly difficult to undertake mitigation measures.

Table 3
Diesel fuel properties used in oil-spill simulations

Viscosity [m Pa s]	Density [kg m^{-3}]	Interfacial tension [mN m^{-1}]	Specific vapour pressure [bar]	Initial boiling point [K]
2	840	28	$3.4\ 10^{-4}$	496

Table 4
Oil-slick area, the remaining oil and evaporation determined with the Nafta3D model

Time [h]	Slick area [1000 m^2]	Spilled oil [t]	Remaining oil [t]	Evaporation [%]
1	427.5	100	66.45	33.5
2	999.1	200	117.7	41.2
3	1485	300	164.9	45.0
5	2653	500	255.9	49.9
10	5667	500	229.9	54.0
20	12723	500	214.1	57.2
40	34044	500	187.5	62.5
70	71067	500	160.8	67.9

Oil concentrations for simulations with and without evaporation in the 30 cm surface layer are shown in Figure 6. The evaporation of each oil-particle is limited, as all particles have the same initial chemical composition. Therefore, the slick area in both simulations does not differ significantly. However, the highest concentrations (thickness) in the core of slicks are two- to threefold higher in simulations without evaporation. In the simulated weather conditions with spatially and temporally variable wind the centre of the slick stays more or less at the same location and the most significant process is the spreading of oil in the dominant wind direction (ENE-WSW).

In a small and environmentally vulnerable area such as the Gulf of Trieste a relatively small 500-ton spill could have devastating consequences for the marine biota and several economic branches dependent on the quality of the marine and coastal environment; fishery, fish-farming and tourism are among the most important. One of the main purposes and benefits of oil-spill models and their application is the support to decision-makers responsible for effective measures following potential oil-spills. On the other hand, one of the main drawbacks of these models is that they are ineffective without adequate input data on circulation. As hydrodynamic simulations are significantly more time-consuming, regular sea-state forecasts for a few days should be available at any time in order to perform oil spill simulations in real time. Such forecasting for the Gulf of Trieste and the Northern Adriatic is in the test phase at the National Institute of Biology and the Slovenian Environment Agency. When the daily sea-state forecasts become available and the Nafta3D model is adequately validated, the model will be used as a reliable support for planning and implementing oil-spill remediation measures.

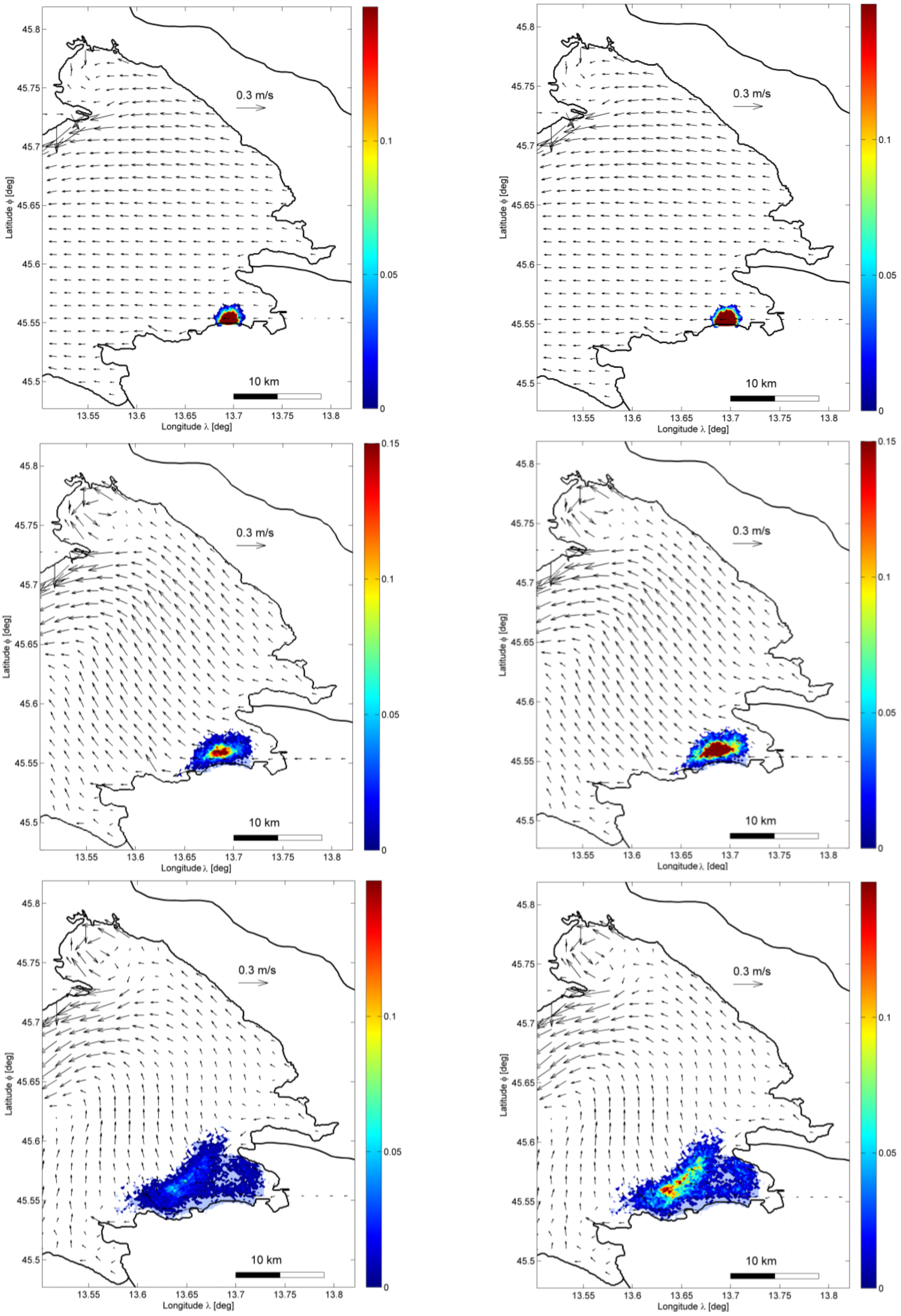

Figure 6: Oil concentrations (kg m^{-3}) in the surface layer at the times 10 h (top), 30 h (middle), and 70 h (bottom) after the spill. Concentrations simulated with (left column) and without evaporation (right column). Velocity fields from real wind in the period 19-21 Mar 2009.

The Nafta3D model has not yet been rigorously validated on an actual oil spill in the area under study, as no such event has been detected. However, validation on a well-documented oil spill in front of the Lebanese coast in 2006 is underway, and the preliminary results show good agreement with satellite observations and other models used for hindcasting of the event (Coppini et al., 2011).

4. *Conclusions*

Several improvements in high-resolution modelling of pollutant dispersion have been introduced during the last few years: the numerical grid was significantly refined; the spatially and temporally averaged input data were replaced with short-term real-time forecasts and reanalyses; and one-way nesting of modelling domains was implemented. Due to the relatively small dimensions of typical contaminated sites, their response time is short and several important transport and transformation processes occur in short time periods (hours). Therefore, the suggested improvements in modelling techniques represent an important step forward in understanding short- and long-term pollutant dispersion and transformation processes.

The implementation of temporal high resolution input parameters enabled the computation of mercury evasion, a previously unknown term in the annual mercury mass balance for the Gulf of Trieste. The spatially variable input data contributed to better understanding of the significant impact of the Soča/Isonzo river plume on mercury contamination in the Baia di Panzano in bora wind conditions. These improvements led to the approach using spatially and temporally variable input data, and one-way nesting of circulation models. An oil-spill model using such high resolution input data can provide valuable information on oil slick propagation and can be used as a support tool in remediation of potential oil spills.

The improved models and modelling approaches can now successfully be used as a support to advanced automatic measurement techniques in contaminated sites. The models and their results have been successfully implemented in the framework of the EU FP7 project “Hydronet”. Simulations of pollutant dispersion and oil spill propagation in the Livorno coastal area and in the Gulf of Trieste were used in aid of mission planning and in the development of a new source-finding algorithm.

Further development of the presented models includes implementation of two-way nesting of modelling domains, sequential one-way nesting (e.g. Mediterranean Sea – Adriatic Sea – Northern Adriatic – Gulf Of Trieste), coupling with atmospheric and surface wave models, and data assimilation using Kalman filters (Korres et al., 2007; Powell et al., 2008; Rozier et al., 2007). These modifications are used in physical oceanography for circulation modelling and should also be applied in transport and dispersion simulations. Further improvements of the BGC module of the PCFLOW3D model should also include more reliable estimations of the parameters influencing mercury transformation processes (oxidation/reduction, biotic/abiotic reduction etc.)

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