Environmental Research 125 (2013) 103–112

Contents lists available at ScienceDirect

Environmental Research

journal homepage: www.elsevier.com/locate/envres

High-resolution pollutant dispersion modelling in contaminated coastal sites

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ARTICLE INFO

Available online 7 March 2013

Keywords:
Mathematical modelling
Hydrodynamic circulation
Pollutant dispersion
Mercury
Evasion
Oil-spill

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.

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).

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0013-9351/$ - see front matter © 2013 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.envres.2012.12.013

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, 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, 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), (2004), Četina et al. (2000), 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 (Fig. 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, 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, 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.

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