Three-dimensional model of radionuclide dispersion in estuaries and shelf seas

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Abstract

The 3-D model THREETOX was developed for the assessment of contamination in coastal seas and inland water bodies. It includes a high resolution numerical hydrodynamic submodel, a dynamic–thermodynamic ice submodel, and submodels for suspended sediment and pollution transport. The results of two case studies are described. The first case concerns a 2-year simulation of the Chernobyl radionuclide contamination of the Dnieper–Bug estuary to validate the model. In the second case study, simulations were performed for the assessment of the consequences of the possible release of radionuclides from scuttled reactors and containers with liquid radioactive wastes in the Novaya Zemlya fjords and the East Novaya Zemlya Trough of the Kara Sea. The simulated results demonstrated the capability of the THREETOX model to describe a wide spatial and temporal range of radionuclide transport processes in the ocean. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords: Numerical simulation; 3-D ocean modelling; Sea ice; Suspended sediment transport; Radionuclide in sea and estuary; Chernobyl radionuclide aquatic transport; Dnieper–Bug Estuary; Black Sea; Kara Sea

Software availability

Program title THREETOX (THREE-dimensional model of TOXicants transport)
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Hardware IBM compatible Pentium 200 or higher; HP Workstation
Program language Fortran
Cost Free ware for researchers

1. Introduction

The use of computational fluid dynamics models is important for operative forecasts of pollutant dispersion in coastal waters and emergency preparedness and response in the case of accidental industrial releases. An advanced THREE-dimensional model of TOXicants transport (THREETOX) was recently developed (Margvelashvili et al., 1997) for the prediction and analysis of pollution transport in coastal seas and inland water bodies.

A brief description of the model is presented and two case studies are considered: a 2-year simulation of the 1986 accidental Chernobyl radionuclide contamination of the Dnieper–Bug Estuary, and a multi-year simulation of a situation caused by a potential radionuclide release from scuttled reactors, and containers with the liquid radioactive wastes, in the Novaya Zemlya fjords and the East Novaya Zemlya Trough in the Kara Sea.
2. Model description

The THREETOX code (Margvelashvili et al., 1997) was used to simulate 3-D hydrodynamics fields, suspended sediments and radionuclide transport. The code includes a set of submodels (Fig. 1).

2.1. Hydrodynamics submodel

The hydrodynamics are simulated on the basis of the 3-D, time-dependent, free surface, primitive equation model. The model equations are written in Cartesian coordinates. The prognostic variables of the hydrodynamics code are the three components of velocity, temperature, salinity and surface elevation. The water body is assumed to be hydrostatic and incompressible. The concept of eddy viscosity/diffusivity and Prandtl’s hypothesis, with the variable turbulence length scale, is used to define the turbulent stresses. At the free surface, all fluxes (momentum, heat, etc.) are prescribed. At the bottom and the land boundaries, the conditions of no diffusive fluxes of any property are used. The open lateral boundary conditions are modified radiation conditions (Blumberg and Kantha, 1985). Sigma co-ordinates were used to reduce difficulties in the numerical solution of the problem for realistic bottom topography. To improve time characteristics of the submodel the barotropic and baroclinic modes split was used in the code (Blumberg and Mellor, 1987).

2.2. Ice submodel

The submodel was developed to simulate the seasonal cycle of moving ice in seas of the temperate zone (Koziy and Maderich, 1997). It is based on the dynamic–thermodynamic model of Hibler (1979, 1980). The submodel describes (1) the momentum balance that defines ice drift induced by wind and currents; (2) the ice rheology, connecting stresses with deformations and strength; (3) the mass balance connecting ice thickness with its growth or loss due to freezing, melting and ice drift; and (4) the ice strength dependent on the size and thickness of floes. The rate of change of momentum was computed from a balance between the wind and water current stresses, Coriolis force, ocean tilt, internal ice stress and inertial terms. The ice rheology is based on a viscous–plastic constitutive law. Ice strength is coupled to ice thickness and compactness, which are changed through advection, convergence or divergence and freezing/melting. Ice thickness distribution is a two-level representation that considers compactness and mean ice thickness, averaged over an entire grid cell.

2.3. Suspended sediment transport submodel

Suspended sediment transport is described by the advection–diffusion equation, taking into account the fall velocity of the sediment grains. The bottom boundary condition describing sediment resuspension or deposition depends on the ratio between equilibrium and actual near bottom suspended sediment concentrations. The van Rijn (1984) approach is used to calculate equilibrium concentration. The thickness of the upper (movable) layer of sediments is governed by the equation of the bottom deformation.

2.4. Radionuclide transport submodel

The equations of radionuclide transport govern the radionuclide concentration in solute, in the suspended sediments and in the top layer of the bottom deposits (Margvelashvili et al., 1997). The exchanges between these variables are described as adsorption–desorption and sedimentation–resuspension processes. 3-D advection–diffusion equations are used to simulate the radionuclide transport in the water column and an ordinary differential equation is applied to simulate the concentration of a radionuclide averaged over the thickness of an upper, mobile layer of bottom deposits. The boundary condition at the water surface is no flux of dissolved and particulate radionuclides. At the bottom boundary the net flux is equal to the sum of fluxes of the particulate and dissolved radionuclides. This approach has been used earlier for 3-D radionuclide marine modelling (Onishi et al., 1989). Important conclusions from the Chernobyl radionuclide data analyses are that there are different distribution coefficient $K_d$ values for the bottom deposits and the suspended sediments, and different rates of sorption and desorption (Zheleznyak, 1997). These facts made it necessary to incorporate the description of the
phenomena in a radionuclide transport submodel. This was tested on the Kiev Reservoir’s data (Zheleznyak and Margvelashvili, 1997).

2.4.1. Water quality submodel

The water quality model, based on the WASP model (Ambrose et al., 1993), is designed for the simulation of eutrophication processes in coastal areas and transport of non-radioactive toxicants.

The explicit–implicit scheme was used for the numerical solution of the momentum equations, advection–diffusion equations for the temperature and salinity, the suspended sediment and radionuclides (in solute and adherent to suspended sediment) transport. Approximation of the advective terms was based on the combination of central and “up-wind” differences. To solve numerically the 2-D system of the ice momentum equations and equations for the thickness and compactness, the method of alternate directions was applied.

3. Case studies

3.1. Dnieper–Bug estuary

The Dnieper–Bug Estuary (DBE), with a surface area of 1006.3 km², and a volume of 4.24 km³, is the largest estuary of the Black Sea, located on its north-west coast (Fig. 2). The Estuary is connected with the Black Sea through the Kinbourn Strait. The regime of this drowned-river estuary varies from stratified to partially mixed. The sources of freshwater discharge are the Dnieper and Southern Bug rivers. The other key factors that govern the transport of pollution are air temperature, wind and sea level variability. Since 1986, the DBE has been the endpoint for radionuclide transport by Dnieper River from the Chernobyl Nuclear Power Plant area to the Black Sea. The radioactive contamination of the DBE offered the opportunity to study the behaviour of dissolved and particulate substances in the transition zone between fresh and salt waters and validate the tracer transport models.

The simulation of the dispersion of radionuclides that entered the DBE after the Chernobyl accident was provided for the period of May 1986–April 1988. To diminish the effect of the uncertainty of sea level elevation at the open boundary, the calculations were carried out in two nested areas. The large area was the whole north-western part of the Black Sea. The temperature, salinity and sea elevation fields from the large area model were used as the open boundary conditions for the nested area shown in Fig. 2. The grid spacing here was 6.0 km in the along-estuary direction, and approximately 3.1 km in the across-estuary direction. The vertical direction was resolved by 15 equally spaced sigma levels. To simulate radionuclide dispersion, the monthly averaged concentrations of sediment, radionuclide in solute and radionuclide adherent to sediment in the Dnieper and Southern Bug mouth, were prescribed from May 1986 to April 1988 using the data of Polikarpov et al. (1988); Kulebakina and Polikarpov (1991); Katrich et al. (1992); Kanivets et al. (1997). At the open sea boundary the concentrations of 137Cs and 90Sr were prescribed according to Batrakov et al. (1994).

Figs. 3 and 4 show, respectively, the simulated vertical distributions of 137Cs and 90Sr along the A–A cross section (see Fig. 2) in July 1987. The difference between the pattern of the 137Cs and 90Sr concentration distributions is clearly visible. The stratification of these radionuclides was opposite. The highest water contamination by 90Sr was inside the DBE, whereas for the 137Cs, water contamination increased seaward. Hence, the DBE was contaminated by 137Cs and purified from 90Sr due to the intrusion of saline water from the Black Sea, and it was contaminated by 90Sr and purified from 137Cs due to the influx of the fresh river water. This can be under-
stood by the difference in self-purification of the Dnieper water from $^{137}$Cs and $^{90}$Sr that flows from the Chernobyl area through a set of reservoirs. As noted by Kanivets et al. (1997), almost all of the riverborne Chernobyl $^{137}$Cs was deposited in the chain of the Dnieper reservoirs. However, only 70% of the $^{90}$Sr was deposited here. Fig. 5 depicts the observed (Polikarpov et al., 1988) and the computed distribution of $^{90}$Sr along the DBE in March 1987. Discrepancies between the observed and the simulated distribution do not exceed the range of uncertainty of the measured values. A more detailed description of the results of the simulation of radionuclide dispersion in the DBE is presented by Margvelashvili et al. (1998).

3.2. Kara Sea

Considerable attention has been focused on the radiological consequences to man as a result of the nuclear reactors and containers with liquid wastes that have been scuttled in the Novaya Zemlya fjords and the Kara Sea by the former Soviet Union. A schematic bottom topography of the Kara Sea and locations of the sites of the potential radionuclide sources are shown in Fig. 6. In the frame of the CEC Study Contract (1997), a numerical simulation was performed to assess the consequences of possible leakage from the dumped reactors and other wastes. The dispersion simulation was carried out consequently on local and regional scales.

The local scale modelling was performed by the THREETOX program, for dump sites in three fjords (Abrosimov, Stepovogo and Tsivolki). Two years of radionuclide dispersion were simulated for the potential releases. Information on the fjords has been obtained from cruise reports (Foyn and Nikitin, 1993, 1994; Joint Russian–Norwegian Expert Group for Investigation of Radioactive Contamination in the Northern Areas, 1996). The CEC Study Contract (1997) scenarios of the release of radioactivity were adopted. Strong seasonal effects on the circulation in the fjords caused by summer run-off from snow melting, and winter ice sheets, in addition to wind and semidiurnal tides were shown. The calculated flushing times ranged from 0.3 months (summer) to 3.4 months (winter) in the relatively small
Stepovogo fjord, to 0.6 and 6.0 months for summer and winter, respectively, in the large Tsivolki fjord.

The distribution of $^{137}$Cs in the Stepovogo fjord in summer (half year after release beginning) is shown in Fig. 7. The east–west spacing of Stepovogo fjord is about 9 km, and north–south spacing is 3.6 km. The typical depth is about 25 m. The inner part of the fjord is relatively deep with the maximum depth of about 50 m. The nuclear submarine NS 601 was dumped in a relatively shallow channel near the bay mouth. A summer fresh water discharge from the western part of the basin results in strong water stratification. The halocline depth at summer is about 15–30 m with a salinity variation of 15‰. As shown in Fig. 7(a), the vertical distribution of $^{137}$Cs in August is inhomogeneous. The concentration of $^{137}$Cs in the mouth increases to the surface whereas in the inner part of the fjord it is maximal near the bottom. It can be explained by the seasonal specifics of the tracer transport in the stratified fjords. During winter the outflux of the radionuclides is relatively weak because ice covers the fjord. An influx of fresh water in July–August "pushes" the contaminated water in the upper layer to the fjord mouth. In the bottom layer the water flows from the sea and transports radionuclides to the inner part of the fjord. Here the contaminated water rises in the upper layer. In Fig. 7(b) the simulated bottom contamination is depicted. The concentration of $^{137}$Cs around the source is much higher than the typical bottom contamination.

Based on the THREETOX estimates of flushing times, a simple box model for the fjords was developed to
extrapolate the results of the 3-D simulation from a few years to 50 years. The box model predicted that, after 50 years since the beginning of a release, the residual amount of $^{137}\text{Cs}$ in the fjords is about 3% from the total input and the average concentration of $^{137}\text{Cs}$ in the water of the fjords didn’t exceed 80 Bq m$^{-3}$.

The area under consideration in the regional scale modelling includes the Kara Sea and the eastern part of the Barents Sea (see Fig. 4). It is about 1240 km long and 1440 km wide. The model resolution was approximately 27 km in the along-basin direction, resulting in 46 grid points, and 27 km in the across-basin direction, providing 53 lateral points. The vertical direction was resolved by 15 levels with the logarithmic stretching of the upper layers. Circulation in the Kara Sea depends on wind field, tidal forcing, river influx, heat balance and mass exchange with other seas (Pavlov, 1994). The monthly wind and air temperature fields from Climate of USSR (Anon., 1980) were used as a forcing in the simulations. The river run-off of Ob and Yenisey was obtained from Pavlov (1994). At the open sea boundaries M$_2$ tide was prescribed. The boundary and initial values of the temperature and salinity fields were specified using the data of the World Ocean Atlas—94 (1994). It was supposed that the sea is ice free at the initial time (1 July). The flux of the radionuclides from the sources in the fjords was calculated by the local box model.

Strong effects of seasonal variability on radionuclide transport in the sea also were revealed. The summer surface current field is given in Fig. 8. The influence of the river inflow on the circulation is clearly visible. The residual tidal current was important in narrows (e.g. Karskie Vorota Strait). The seasonal changes of the water exchange with the Barents Sea and the Arctic Ocean

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**Table 1**

Flows through the Kara Sea boundaries (1 Sv = 10$^6$ m$^3$ s$^{-1}$)

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<tbody>
<tr>
<td>Barents Sea–Kara Sea</td>
<td>0.15</td>
<td>0</td>
<td>(0.04–0.6)</td>
<td></td>
<td>0.6</td>
</tr>
<tr>
<td>(Karskie Vorota Strait)</td>
<td></td>
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<tr>
<td>Arctic Ocean–Kara Sea</td>
<td>–1.51</td>
<td>–1.89</td>
<td>–0.15–0.54</td>
<td>–1.6</td>
<td>–0.63</td>
</tr>
<tr>
<td>Barents Sea–Kara Sea</td>
<td>1.33</td>
<td>1.89</td>
<td>0.6–0.7</td>
<td>1.2</td>
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were much more than the mean year. Simulated mean year net fluxes through the open boundaries of the Kara Sea are shown in Table 1. Comparison with the available data from different literature sources shows that the simulated year averaged fluxes did not exceed the uncertainty of the reported data. The $^{137}\text{Cs}$ distributions at the sea surface, after 1 and 8 years since the start of a release are depicted in Fig. 9. The radionuclide flow is directed towards both the Barents Sea and the Arctic Ocean. It should be noted here that the natural level of the Kara Sea water contamination is about 3 Bq m$^{-3}$, while the simulated level of contamination due to the release of radionuclides from the dump sites is less than 0.2 Bq m$^{-3}$.

4. Summary

The 3-D model, THREETOX, was developed for the assessment of real and potential emergency situations of toxic releases in the coastal areas of seas and inland water bodies. It includes a high resolution numerical hydrodynamic submodel, a dynamic–thermodynamic ice submodel, and submodels for suspended sediment, water quality and pollution transport. The results of two case studies have been described.

The first one concerns a 2-year simulation of the Chernobyl radionuclide transport through the Dnieper–Bug Estuary into the Black Sea to validate the model. The simulation results were in reasonable agreement with the available data.

In the second case study, simulations were carried out for the assessment of a potential emergency situation caused by radionuclide release from scuttled reactors and containers with liquid radioactive wastes in the Novaya Zemlya fjords and the East Novaya Zemlya Trough. Strong effects of seasonal variability on radionuclide transport were revealed, both in the fjords and in the sea. Based on the results from the THREETOX simulations, a simple box model for the fjords was developed to extrapolate the results of the 3-D simulation from a few
years to 50 years. It was predicted that, after 50 years since the beginning of a release, the residual amount of \(^{137}\text{Cs}\) in the fjords is about 3% from the total input. The calculations showed that the average concentration of \(^{137}\text{Cs}\) in the fjords would not exceed 80 Bq m\(^{-3}\). The simulated level of contamination in the Kara Sea due to the release of radionuclides from dump sites is less than 0.2 Bq m\(^{-3}\), whereas the natural level of the Kara Sea water contamination is about 3 Bq m\(^{-3}\).

The simulated results demonstrated the capability of the THREETOX model to describe a wide spatial and temporal range of transport processes in the ocean.

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