
Modelling the radionuclide contamination of the Black Sea in the result of Chernobyl accident using circulation model and data assimilation

S. Yuschenko, I. Kovalets, V. Maderich, D. Treebushny and M. Zheleznyak

Institute of Mathematical Machine and System problems, Glushkov Av. 42, 03187 Kiev, Ukraine, e-mail: sergey@env.kiev.ua

Abstract. Assimilation of observations is a powerful tool to improve the predictive capabilities of models for radionuclide transport and fate. We describe results of numerical experiments on assimilation of the data on radionuclide contamination of the Black Sea in the result of Chernobyl accident using the three-dimensional model of circulation and radionuclide transport THREETOX. Data assimilation can be formulated as a procedure that contains two steps: update and forecast. On the update step THREETOX is run from the time of release or deposition to the time of the forecast using the updated input from all the measured data available at this period to be assimilated. On the forecast step THREETOX is run from the forecast time to the end of the modeling period using the results of the update step to produce the forecast of radionuclide transport. The data assimilation method called "method of iterations to optimal solution" (IOS) was used at the update step. The approach has been applied to the assimilation of the observational data of ^{137}Cs concentration measured in the "Typhoon" surveys for the period June 1986 to September 1990. From the results of numerical experiments we conclude that usage of a data assimilation procedure can essentially improve predictive capability of the models for radionuclide transport. The computational time for the data assimilation method chosen is small in comparison with the general time of calculations. Results from the study will provide a better understanding of the processes of radionuclide transport in the seas. This novel approach was implemented in the EU DSS RODOS for the real-time simulation of radioactivity transport in the marine environment.

1. INTRODUCTION

Area of the Black Sea was polluted because of the south trace of Chernobyl radioactive cloud. The first systematical observations of the radionuclide concentrations took place from 12 June to 4 July 1986. The radioactive contamination in the Black Sea waters was studied using different approaches. However they still not cover sufficiently all directions of impact and relative details. There is lack of comparable and systematically collected data for the whole basin. The available data are from several expeditions held after the Chernobyl accident. These were organized by the institutions from the former USSR: "Typhoon", IBSS, MHI, Hydro-Meteorological Service as well as several US-Turkey expeditions on the RV "K. Piri" and "Knorr". None of them covered the entire area of the basin. The data from the deeper layers (below the surface layer) were very irregular and scarce. The RER/2003 IAEA TC Project "Marine Environmental Assessment of the Black Sea Region" marked a promising start allowing to obtain a broader and comparable data sets.

The consequences of the Chernobyl accident for the entire coast of Europe revealed the necessity to study the radioactive contamination and its time-spatial evolution. In [1] the coupled system of 3D hydrodynamics model THREETOX and radiological box model POSEIDON/RODOS was applied to the Black Sea for reconstruction and estimation of ^{137}Cs and ^{90}Sr contamination in the result of Chernobyl accident. These models were implemented in the European system RODOS for emergency response to nuclear accident [1] for the forecast of the radioactive contamination in the case of accidental fallout of radioactivity on the surface of the water body. The first experience of the

operational use of the RODOS system showed a strong need in the development of the data assimilation tools for the prognostic models used in RODOS [3]. That was connected with the fact, that with time after release the measurements data of radionuclide concentrations, gamma dose rates, etc. become available to the users of RODOS. At the same time the prognostic models of RODOS usually started their calculations beginning from the time of the release and were not designed to use these measured data. The use of measured data in the calculations of prognostic models is known as the problem of data assimilation. In the frames of the EU DAONEM project data assimilation tools were developed for the most of RODOS prognostic models, including the models of the hydrological model chain [4]. A set of specific constraints for the data assimilation in real-time system [4] were the main factors in choosing the particular method of data assimilation. Among them the strongest constraint is the operational applicability of the chosen method.

Data assimilation (DA) methods in oceanography and meteorology were comprehensively reviewed in many publications (e.g., [5]). These methods can be divided into two main classes: sequential data assimilation and variational data assimilation. Sequential approach is used to estimate the state of system by combining measurements, dynamical model and empirical principles. Explicit definition of the noise statistics of model and data uncertainties is necessary. General sequential approach for the discretized models is the Kalman filter (KF) [5]. KF for linear systems is optimal in the sense of minimum variance state estimate. Different known algorithms of DA (nudging, optimal interpolation) are simplified variants of suboptimal schemes based on KF. Another approach is variational data assimilation algorithm that performs global time/space adjustment of the model solution to the full set of available observations. Both approaches have advantages and disadvantages. For the real time system it is important that in the sequential DA every individual observation is being used only once without feedback to the past, whereas variational approach needs to readjust previous system states.

Data assimilation in THREETOX was formulated as a procedure that contains two steps: update and forecast. On the update step THREETOX is run from the time of release or deposition to the time of forecast using an updated input from the hydrological model chain and all the measured data available at this period that can be assimilated. On the forecast step THREETOX is run from the forecast time to the end of the modeling period using the results from the update step to produce the forecast of radionuclide transport. The method of DA chosen for the THREETOX model is based on the IOS method [7]. The brief description of the THREETOX model and the method of data assimilation are given in the paper. Application results of the described methodologies to calculation of the radionuclide distribution in the Black Sea are presented.

2. DESCRIPTION OF METHODOLOGY

THREETOX model is an advanced three-dimensional surface water modeling system for hydrodynamic and radionuclides transport in lakes, reservoirs, estuaries and the coastal ocean. It has been developed as a part of RODOS system. The code of THREETOX includes a set of submodels: hydrodynamics submodel, suspended sediment transport submodel and radionuclide transport submodel. Hydrodynamics is simulated on the basis of three-dimensional, time-dependent, free surface, primitive equation model [6]. The prognostic variables of the hydrodynamics code are three components of velocity, temperature, salinity and surface elevation. Suspended sediment transport is described by advection-dispersion equations, taking into account fall velocities of sediment grains. Bottom boundary condition describes sediment resuspension or settling down depending on the ratio between equilibrium and actual near bottom suspended sediment concentration. The thickness of bottom deposition upper layer is governed by the equation of bottom deformation. The equations of radionuclide transport describe concentrations of radionuclide in the solute phase, suspended sediment phase and in bottom deposition. Exchanges between these forms are described as adsorption-desorption and sedimentation-resuspension processes. Equations of the THREETOX model are solved with the data assimilation method.

After testing the various methods of data assimilation the method of “iterations to optimal solution”(IOS) was chosen. The method has been suggested in [7] and was applied in atmospheric models [8]. As it was shown in [7] the IOS procedure is close to the well known “optimal interpolation” method. In the IOS algorithm the fields of concentration $\hat{C}_s^w(X, t)$ are updated using data of observations in points $r = 1, \dots, N$ for time $t = t_i$ by the iteration cycle:

$$\hat{C}_s^{w(n+1)}(X_i, t_l) = \hat{C}_s^{w(n)}(X_i, t_l) + (1 + q_i)^{-1} \sum_{r=1}^N \left(\frac{\sigma_B^2}{\sigma_O^2} \right) w(X_{ir}) [C_s^{wobs}(X_r, t_l) - \hat{C}_s^{w(n)}(X_r, t_l)] \quad (1)$$

$$+ (1 + q_i)^{-1} [C_s^{w(0)}(X_i, t_l) - \hat{C}_s^{w(n)}(X_i, t_l)]$$

$$q_i = \sum_{r=1}^N \left(\frac{\sigma_B^2}{\sigma_O^2} \right) |w(r_{ir})|, \quad (2)$$

where

n is the number of iterations,

$\hat{C}_s^{w(0)}(X, t)$ is the first guess concentration field before iteration procedure,

$C_s^{wobs}(X_r, t_l)$ is the measured concentration of the radionuclide in the spatial points $r = 1, \dots, N$ for the point of time $t = t_l$,

R_{cor} is the radius of influence,

σ_B^2 / σ_O^2 is the ration of the mean square deviation of the first guess field $C_s^w(X, t)$, to the mean square observation error.

The weight function $w(X_k - X_i) = w(X_{ik})$ is the correlation function of the deviations of the true field from the first guess field which is selected so that $w(X_k - X_i) = 1$ when $X_k = X_i$ and $w(X_k - X_i) \rightarrow 0$ as $|X_k - X_i| \rightarrow \infty$. We choose $w(X_k - X_i)$ as:

$$w(X_k - X_i) = \exp\left(-\frac{r_{ik}^2}{2R_{cor}^2}\right), r_{ik} = \sqrt{(x_k^2 - x_i^2) + (y_k^2 - y_i^2)} \quad (3)$$

The strong sides of the IOS method are the following: (1) it almost does not require additional computational time that is highly important for the needs of the real time decision support systems like RODOS; (2) it requires the estimates of the relative error σ_B^2 / σ_O^2 only but not the absolute values of the σ_B and σ_O ; (3) it preserves the main properties of the suboptimal schemes based on KF, such as optimal interpolation. The last means, that for the vectors of observations and of the first guess field \mathbf{f}_O and \mathbf{f}_B of the quantity \mathbf{f} measured at the same set of points $0 < k < K + 1$, with $K \times K$ covariance matrices $\underline{\mathbf{O}} = \langle (f_O^i - f^i) \cdot (f_O^j - f^j) \rangle$, $\underline{\mathbf{B}} = \langle (f_B^i - f^i) \cdot (f_B^j - f^j) \rangle$, $0 < i, j < K$ the procedure (1)-(2) minimizes the cost functional:

$$\mathbf{f}_A = \mathbf{f}_B + \underline{\mathbf{B}}[\underline{\mathbf{B}} + \underline{\mathbf{O}}]^{-1} [\mathbf{f}_O - \mathbf{f}_B] \quad (4)$$

if the parameter σ_B^2 / σ_O^2 is constant in domain and the covariance matrix $\mathbf{O}(i, j)$ can be approximated as $\mathbf{O}(i, j) \approx \sigma_B^2 w(i, k)$, where $w(i, k)$ is defined by relationship (3). The same functional (4) is minimized in the KF approach, however, assumptions on the background error covariance matrix $\mathbf{O}(i, j)$ in the KF approach are not restricted to those used here.

The whole data assimilation cycle consists of two steps. At the “forecast” step the calculation of first guess concentration field is performed with the finite-difference approximations of equation of the concentration transport between times of observations. At the “correction” step the values of the first guess field are updated using the algorithm (1)-(3).

As the IOS method was originally designed for the relatively homogeneous fields of the concentration, then if the field of concentration is essentially non-homogeneous (for instance, in short time after the concentration fallout on the surface of the water pond) the special measures should be

taken to prevent the appearance of the negative values of concentrations. The simplest way is to perform the data assimilation cycle only in the points where the concentration values are not less than the certain fraction of the maximum concentration in domain: $C(x_i) > 0.1C_{\max}$.

3. CALCULATION RESULTS

For calculation of the radionuclide distribution in the Black Sea the bottom topography is interpolated to the model grid from 27.7×23 km with the general number of points 50×30 . The model resolves the vertical stratification using 21 vertical levels on the sigma coordinate system. The minimal depth of the shelf is set to 10m. The mean month wind stress field were derived from Hellerman and Rosenstein monthly climatology's database; the data of wind stress components and temperature of air are interpolated on the model grid. The climatological seasonal fluxes of water of Danube and Dniepr Rivers were used. The Bosphorus Strait is modeled as hydraulic two layer system in one grid point: inflow in bottom layer from Sea of Marmara and the outflow in top layer. The fields of velocity, temperature, salinity and radionuclide over a period of time with January 1986 on December 1991 were calculated with temporal resolution 20 min.

On the Figure 1 the distribution of ^{137}Cs in the surface layer in June 1986, reconstructed from measurements [9] after Chernobyl fall-out is depicted. Results of numerical experiments of the data assimilation for Black Sea are shown in Figure -Figure . The radius of influence $R_{\text{cor}} = 60\text{km}$ was used for calculation of matrix correlation function (3). Observations marked with diamonds were used for procedure of assimilation, observations marked in squares were used for calculation of the root mean square error.

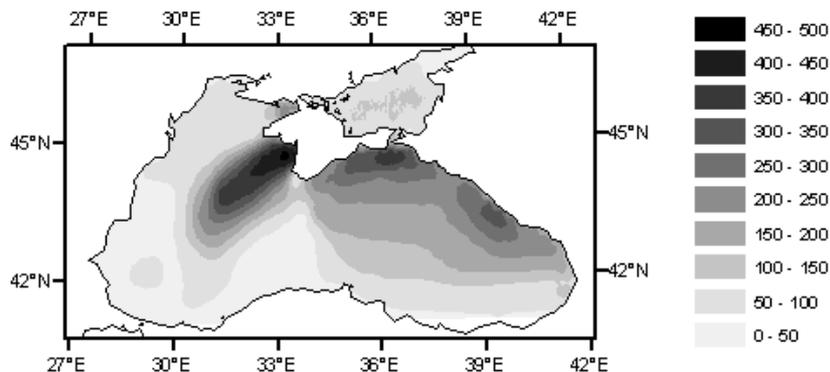


Figure 1. Concentration ^{137}Cs (Bq/m^3) in the surface layer after Chernobyl fall-out, June 1986.

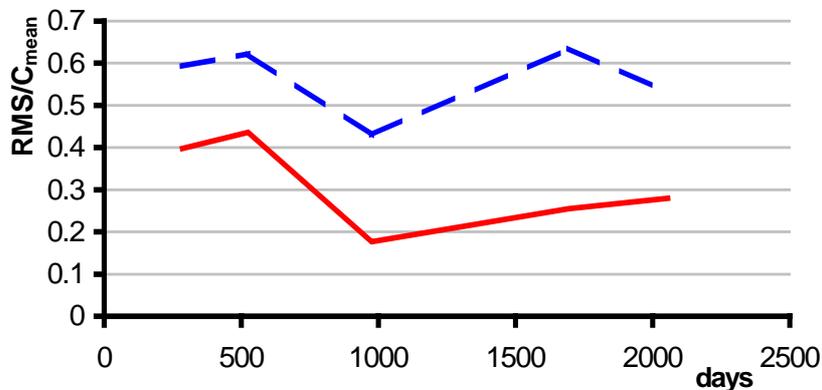


Figure 2. Evolution of the root mean square error: dashed line – without DA, solid line – with DA.

At the Figure the relative root mean square errors (RMS) $\delta = \sqrt{\sum_{i=1}^n \frac{1}{n} (C_m^i - C_{obs}^i)^2} / \sum_i \left(\frac{1}{n} C_{obs}^i\right)$ of the forecasts with and without the data assimilation are shown. As it can be seen from the Figure the effect of DA on the quality of the predicted radionuclide concentrations is increasing with time for the period from the start of calculations to the time $t \approx 1000$ days. For the times $t > 1000$ days the relative error δ of the radionuclide field calculated with DA is approximately 2 times better than δ of the radionuclide field calculated without DA. The values of the absolute RMS error $\delta_1 = \sqrt{\sum_{i=1}^n \frac{1}{n} (C_m^i - C_{obs}^i)^2}$ calculated with the use of the DA are less than the values of the δ_1 calculated without DA by the value from 10 to 20 Bq/m³.

Calculated without the use of data assimilation 3D fields of the radionuclide concentrations presented on Figure 3, Figure show the high maximum of the radionuclide concentrations in the middle of the Black Sea. It decreases on the pictures where the results of calculations with the data assimilation are presented. The locations of maximum values are displaced under the influence of DA.

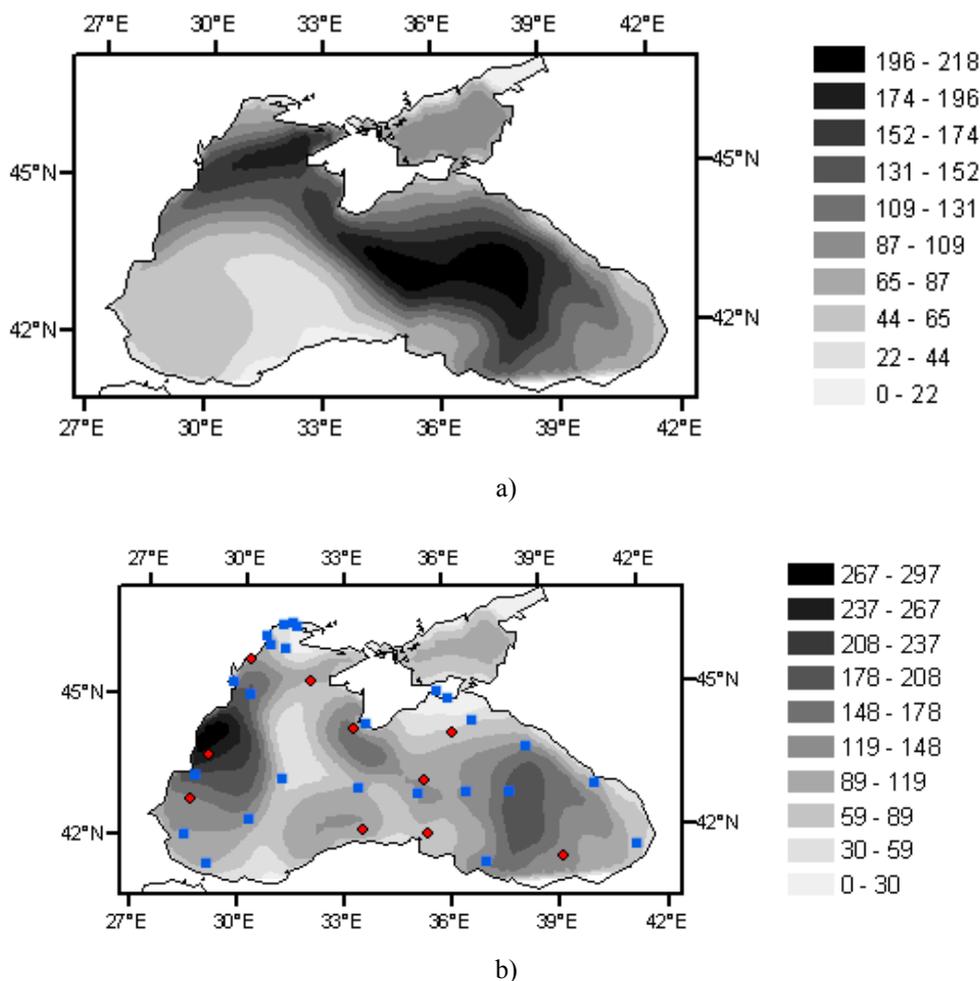


Figure 3. Concentration ¹³⁷Cs in the surface layer of Black Sea, October 1986, Bq/m³: a) without data assimilation; b) with data assimilation approach.

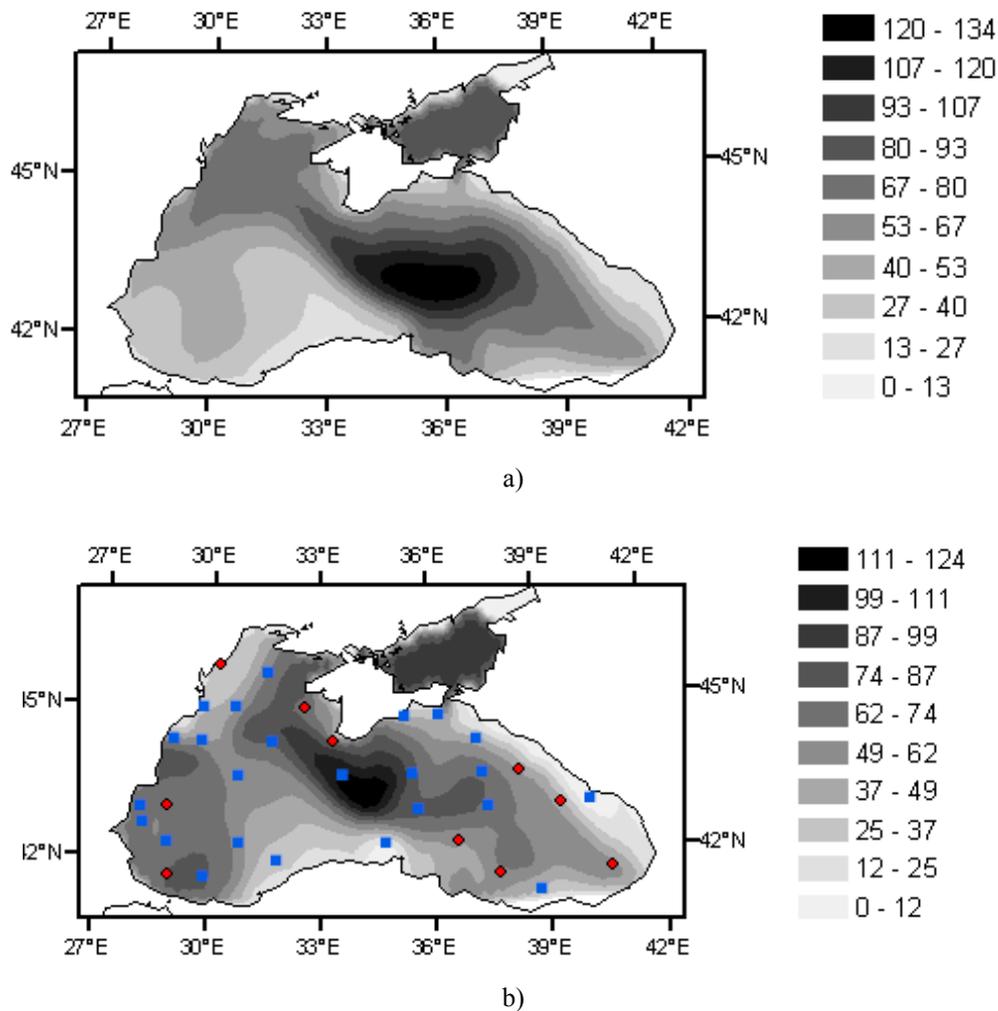


Figure 4. Concentration of ^{137}Cs in the surface layer of Black Sea, June 1987, Bq/m³: a) without data assimilation; b) with data assimilation.

4. CONCLUSIONS

From the results of numerical experiments we can conclude, that the method of iterations of optimal solution can be used for the real-world problem of data assimilation for the calculation of the radionuclide concentration in 3-D model THREETOX. The method performs better for more smoothly distributed concentration fields.

Acknowledgements

The presented work has been fulfilled in the frames of the FP5 EU project DAONEM, Contract No FIKR-CT-2000-0025.

References

- [1] Koziy L., Maderich V., Margvelashvili N., Zheleznyak M., *J. Environmental Modeling and Software*, **13** (5/6), (1998), 413-420.
- [2] J. Ehrhardt, *Radiat. Prot. Dosimetry*, **73**, 1997, 41-44.
- [3] M. Ahlbrecht, R. Borodin, V. Borzenko, J. Ehrhardt, S. French, V. Shershakov, A. Sohler, E. Traktengerts, and A. Verbruggen, *Radiat. Prot. Dosimetry*, **73**, (1997), 81-84.
- [4] C. Rojas-Palma, H. Madsen, F. Gering, R. Puch, C. Turcanu, P. Astrup, H. Müller, K. Richter, M. Zheleznyak, D. Treebushny, M. Kolomeev, D. Kamaev, and H. Wynn, *Radiat. Prot. Dosimetry*, **104**, (2003), 31-40.
- [5] Robinson A.R., Lermusiaux P.F.J., Sloan N.Q., "Data Assimilation". In: *The Sea*, V. 10, eds. H. Brink, A. Robinson. John Wiley & Sons, (1999), pp.541-593.
- [6] N. Margvelashvili, V. Maderich, and M. Zheleznyak, *Radiat. Prot. Dosimetry*, **73**, (1997) 177-180.
- [7] Daley R. *Atmospheric Data Analysis*, Cambridge University Press, (1999), 455pp.
- [8] I. Kovalets, S. Andronopoulos, J. Bartzis, , N. Gounaris, A. Kushchan, *Atmospheric Environment*, **38/3**, (2004), 457-467
- [9] B. Veleva, I. Koziy, S. Yushchenko, V. Maderich, G. Mungov, *Radioprotection-Colloques*, **37-C1**, (2002), 827-832