THE RISK ANALYSIS IN COASTAL ZONE USING REVERSE-TIME DIFFUSION

D. SPIVAKOVSKAYA[1], A.W. HEEMINK[1], J.G.M. SCHOENMAKERS[2]

[1]Faculty of Electrical Engineering, Mathematics and Computer Science,
Department of Applied Mathematical Analysis, Delft University of Technology,
Mekelweg 4, 2628 CD Delft, The Netherlands
[2] Weierstrass Institute for Applied Analysis and Stochastics,
Mohrenstrasse 39, D-10117 Berlin, Germany

Abstract

In this paper we investigate the risk of very high concentrations of pollutants in coastal waters. The method to construct the risk map is based on the concept of reverse time diffusion. Using the reverse time model, which can be derived from the original one, we can simulate backward particle trajectories. By averaging the results of many independent realizations of the reverse time model we can build the risk map. Comparing with the direct Monte-Carlo method based on the original random walk models, the proposed method is more attractive from the computational point of view. In this paper we apply the reverse time method to investigate the risk at critical locations along Dutch seaside and construct risk maps for the Dutch coastal zone.

1. INTRODUCTION

Last several years we have been faced with serious ecological problems due to calamities at sea. As a result a number of problems connected with the transport of the pollutant have arisen. For instance, it is very important to be able to predict accurately the mean and the standard deviation of the concentration of the pollutant at certain areas some time after the release. There are two main approaches to solve these kinds of problems. One can adopt the Eulerian approach and solve the advection-diffusion equation using one of the numerical schemes available. Another method is to interpret the advection-diffusion equation as a Fokker-Planck equation and derive the system of stochastic differential equations for the behavior of one particle of the pollutant. By numerical integrating of this system it is possible to simulate the positions of many particles of the pollutant and describe the pollution process [Heemink, 1990, Spivakovskaya et. al, 2005].

Another problem is connected with the simulation of the reverse pollution process. Suppose that for some critical locations a high concentration of the pollutant can be dangerous or even fatal for life of some species. To prevent ecological disasters we need to determine which areas in the sea are potentially dangerous for the critical location and which areas are safe, in other words we need to construct a risk map. By the risk map for a given location of interest along the coast we mean the concentration of the pollutant in this area for any locations $\boldsymbol{x} = (x_1, x_2)$ where the pollutant may be released. From a risk

map we can immediately determine the most dangerous as well as the safe location of the pollutant release. One of the most effective approach to solve this problem is to use the reverse time particle models based on the solution of the backward Kolmogorov equation [Anderson, 1982, Elliott and Anderson, 1985, Sabelfeld and Shalimova, 2001].

In this paper we use the reverse time system of stochastic differential equations that can be derived from the original one [Milstein et al., 2004, Kurbanmuradov et al., 1992] for the simulation of the transport of the pollutant in reverse time. Several critical locations along Dutch seaside are examined and the risk maps for different moments of time are constructed.

2. PARTICLE MODEL FOR THE ESTIMATION CONCENTRATION IN SHALLOW WATER

The concentration of the pollutant $C(t, \boldsymbol{x}, s, \boldsymbol{z})$, $t \le s \le T$ released at time t at location $\boldsymbol{x}$ can be found from the well-known vertically-integrated advection-diffusion equation [Fischer et al., 1979, Singh and Hager, 1996]

$$\begin{aligned} &\frac{\partial (CH)}{\partial s} + \frac{\partial (u_1 HC)}{\partial z_1} + \frac{\partial (u_2 HC)}{\partial z_2} = \frac{\partial}{\partial z_1}\left(HD \frac{\partial C}{\partial z_1} \right) + \frac{\partial}{\partial z_2}\left(HD \frac{\partial C}{\partial z_2} \right), \\ &C(t, \boldsymbol{x}; t, \boldsymbol{z}) = \delta(\boldsymbol{x} - \boldsymbol{z}), \end{aligned} \tag{1}$$

where $\boldsymbol{x}, \boldsymbol{z} \in \mathbb{R}^2$, H is water depth, D is dispersion coefficient and $\boldsymbol{u} = (u_1, u_2)^T$ is velocity vector.

By substituting the probability density function $p = HC$ to find a particle in certain location we can interpret the equation (1) as a Fokker-Planck equation and derive the consistent system of stochastic differential equations in Îto sense [Heemink, 1990, Spivakovskaya et. al, 2005]

$$\begin{aligned} &d\boldsymbol{X}(s) = \left(\boldsymbol{u} + \frac{D}{H}\frac{\partial H}{\partial \boldsymbol{z}} + \frac{\partial D}{\partial \boldsymbol{z}} \right) ds + (\sqrt{2D}\boldsymbol{I}_2) d\boldsymbol{W}(s), \\ &\boldsymbol{X}(t) = \boldsymbol{x}, \end{aligned} \tag{2}$$

where $\boldsymbol{X} = (X_1, X_2)^T$ is 2-dimensional stochastic process, $\boldsymbol{W} = (W_1, W_2)^T$ is 2-dimensional Brownian motion, $\frac{\partial}{\partial \boldsymbol{z}} = \left(\frac{\partial}{\partial z_1}, \frac{\partial}{\partial z_2} \right)^T$ is the spatial variation vector and $\boldsymbol{I}_2$ is the 2×2 identity matrix. If the initial location $\boldsymbol{x}$ of the release of the pollutant is known, we can simulate the positions of many particles using the numerical solution of the system (2) and find the probability density function $p(t, \boldsymbol{x}, s, \boldsymbol{z})$ (and correspondingly the concentration $C(t, \boldsymbol{x}, s, \boldsymbol{z})$).

In the most applications the initial time t and location of the release $\boldsymbol{x}$ are known and our goal is to find the concentration of the pollutant in some point $\boldsymbol{y}$ at the time T. Let us consider now the opposite problem: we fix the end location $\boldsymbol{y}$ and time T and consider the function $C(t, \boldsymbol{x}, T, \boldsymbol{y})$ as a function depending on variables t and $\boldsymbol{x}$. This function may be interpreted as a risk map. We can find the critical locations of the release of the pollutant $\boldsymbol{x}$ for the location $\boldsymbol{y}$ (or for which locations $\boldsymbol{x}$ the concentration $C(t, \boldsymbol{x}, T, \boldsymbol{y})$ may exceed a dangerous value). Besides, such risk map can help us to find the location of the release of the pollutant if we know the concentration in some location.

3. REVERSE-TIME ESTIMATOR

First of all, let us consider the stochastic differential equation in the Îto sense in general form:

$$\begin{aligned} &d\boldsymbol{X}(s) = \boldsymbol{a}(s,\boldsymbol{X})ds + \boldsymbol{\sigma}(s,\boldsymbol{X})d\boldsymbol{W}(s), \quad t \le s \\ &\boldsymbol{X}(t) = \boldsymbol{x} \end{aligned} \tag{3}$$

where $\boldsymbol{X} = (X_1, \ldots, X_d)^T$. $\boldsymbol{a} = (a_1, \ldots, a_d)^T$ are d-dimensional vectors, $\boldsymbol{W} = (W_1, \ldots, W_m)^T$ $(m \ge d)$ is a m-dimensional Wiener process and $\boldsymbol{\sigma} = \{\sigma_{ij}\}$ is a $d \times m$ matrix. We assume that the $d \times d$ matrix $\boldsymbol{b} = \boldsymbol{\sigma}\boldsymbol{\sigma}^T$ is of full rank for every $(s, \boldsymbol{z})$, $s \in [t, T]$, $\boldsymbol{z} \in \mathbb{R}^d$. We also assume that the functions $a_i(s, \boldsymbol{z})$ and $\sigma_{ij}(s, \boldsymbol{z})$ and their first derivatives are continuous and bounded. This particularly implies existence and uniqness of the solution $\boldsymbol{X}_{t,\boldsymbol{x}}(s) \in \mathbb{R}^d$, $\boldsymbol{X}(t) = \boldsymbol{x}$ of (3), smoothness of the transition density $p(t, \boldsymbol{x}, s, \boldsymbol{z})$ of the Markov process $\boldsymbol{X}$ and existence of all the moments $p(\cdot, \cdot, \cdot, \boldsymbol{y})$ [Arnold, 1974, Oksendal, 1985, Jazwinski, 1970].

The probability density function $p(t, \boldsymbol{x}, s, \boldsymbol{z})$ of the system (3) satisfies the Fokker-Planck (or Kolmogorov forward) equation $(t \le s)$

$$\begin{aligned} &\frac{\partial p}{\partial s} = \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2}{\partial z_i \partial z_j}(b_{ij}p) - \sum_{i=1}^{d} \frac{\partial}{\partial z_i}(a_i p), \\ &p(t, \boldsymbol{x}, t, \boldsymbol{z}) = \delta(\boldsymbol{x} - \boldsymbol{z}) \end{aligned} \tag{4}$$

In order to find the probability density function $p(t, \boldsymbol{x}, T, \boldsymbol{y})$ we can use the standard method of non-parametric statistics called kernel estimator [Wand and Jones, 1995].

$$\widehat{p}(t, \boldsymbol{x}, T, \boldsymbol{y}) = \frac{1}{N\delta^d} \sum_{n=1}^{N} K\left(\frac{\overline{\boldsymbol{X}}_{t,\boldsymbol{x}}^{(n)} - \boldsymbol{y}}{\delta}\right), \tag{5}$$

where $\left\{\overline{\boldsymbol{X}}_{t,\boldsymbol{x}}^{(n)}\right\}$, $n = 1, \ldots, N$ are independent realizations of the stochastic process $\overline{\boldsymbol{X}}_{t,\boldsymbol{x}}$ and $\overline{\boldsymbol{X}}_{t,\boldsymbol{x}}$ is the approximation of the stochastic process $\boldsymbol{X}$ started at point $\boldsymbol{x}$ at time t. Because the estimator (5) is based on the forward system (3) it is often called forward estimator (FE). The forward estimator is not efficient for risk analysis, because we need to simulate the realizations of the stochastic process $\overline{\boldsymbol{X}}_{t,\boldsymbol{x}}$ for different initial conditions $\boldsymbol{x}$. The more efficient method is a reverse-time approach.

Let us introduce a reverse-time variable $\tilde{s} = T + t - s$ and define the functions

$$\begin{aligned} &\tilde{a}_i(\tilde{s}, \boldsymbol{z}) = a_i(T + t - \tilde{s}, \boldsymbol{z}), \\ &\tilde{b}_{ij}(\tilde{s}, \boldsymbol{z}) = b_{ij}(T + t - \tilde{s}, \boldsymbol{z}) \\ &\tilde{\sigma}_{ij}(\tilde{s}, \boldsymbol{z}) = \sigma_{ij}(T + t - \tilde{s}, \boldsymbol{z}) \\ &\tilde{p}(\tilde{s}, \boldsymbol{z}, T, \boldsymbol{x}) = p(t, \boldsymbol{x}, T + t - \tilde{s}, \boldsymbol{z}) \end{aligned} \tag{6}$$

By substituting the variable $\tilde{s}$ in the equation (4) it can be rewritten in the form

$$\begin{aligned} &\frac{\partial \tilde{p}}{\partial \tilde{s}} = -\frac{1}{2}\sum_{i,j=1}^{d} \tilde{b}_{ij} \frac{\partial^2 \tilde{p}}{\partial z_i \partial z_j} - \sum_{i=1}^{d} \alpha_i \frac{\partial \tilde{p}}{\partial z_i} - c(\tilde{s}, \boldsymbol{z})\tilde{p}, \\ &\tilde{p}(T, \boldsymbol{z}; T, \boldsymbol{x}) = \delta(\boldsymbol{z} - \boldsymbol{x}) \end{aligned} \tag{7}$$

where

$$\begin{aligned} \alpha_i(\tilde{s}, \boldsymbol{z}) &= \sum_{j=1}^{d} \frac{\partial \tilde{b}_{ij}}{\partial z_j} - \tilde{a}_i, \\ c(\tilde{s}, \boldsymbol{z}) &= \frac{1}{2} \sum_{i,1=1}^{d} \frac{\partial^2 \tilde{b}_{ij}}{\partial z_i \partial z_j} - \sum_{i=1}^{d} \frac{\partial \tilde{a}_i}{\partial z_i} \end{aligned} \tag{8}$$

It can be proved [Milstein et al., 2004, Kurbanmuradov et al., 1992] that the solution of the equation (7) can be represented in the form

$$\tilde{p} = E\left[g\left(\boldsymbol{Y}_{t,\boldsymbol{y}}(T)\right)\mathcal{Y}_{t,\boldsymbol{y}}(T)\right], \tag{9}$$

where $g(\boldsymbol{u}) = \delta(\boldsymbol{x} - \boldsymbol{u})$ is a delta function and $(\boldsymbol{Y}, \mathcal{Y})$ is the solution of the following system of the stochastic differential equations called reverse-time system

$$\begin{aligned} &d\boldsymbol{Y} = \boldsymbol{\alpha}(\tilde{s}, \boldsymbol{Y})d\tilde{s} + \tilde{\boldsymbol{\sigma}}(\tilde{s}, \boldsymbol{Y})d\tilde{\boldsymbol{W}}(\tilde{s}), \\ &d\mathcal{Y} = c(\tilde{s}, \boldsymbol{Y})\mathcal{Y}ds, \\ &\boldsymbol{Y}(t) = \boldsymbol{y}, \quad \mathcal{Y}(t) = 1 \end{aligned} \tag{10}$$

For the sake of simplicity the tildes will be dropped. In the most cases the system (10) can not be solved analytically. Suppose that $(\overline{\boldsymbol{Y}}, \overline{\mathcal{Y}})$ is a numerical solution of (10) received by using one of the numerical schemes (for instance, Euler scheme) [Kloeden and Platen, 1992, Milstein and Tretyakov, 2004]. Then, by applying the kernel estimator it is possible to construct the following estimator

$$\widehat{p}(t, \boldsymbol{x}, T, \boldsymbol{y}) = \frac{1}{M\delta^d} \sum_{m=1}^{M} K\left(\frac{\boldsymbol{x} - \overline{\boldsymbol{Y}}_{t,\boldsymbol{y}}^{(m)}}{\delta}\right) \overline{\mathcal{Y}}_{t,\boldsymbol{y}}^{(m)}(T), \tag{11}$$

where $(\overline{\boldsymbol{Y}}_{t,\boldsymbol{y}}^{(m)}, \overline{\mathcal{Y}}_{t,\boldsymbol{y}}^{(m)})$, $m = 1, \ldots, M$ is an independent identically distributed (i.i.d.) sample of numerical solution of (10), δ is a bandwidth, K is kernel function. The estimator (11) is known as reverse estimator (RE).

The accuracy of the both forward estimator (5) and the reverse estimator (11) depends on the choice of the kernel function K and the bandwidth δ. It is well known [Silverman 1986, Wand and Jones, 1995] that the optimal choice for the bandwidth is given by

$$\delta = \mathcal{O}\left(N^{-\frac{1}{4+d}}\right). \tag{12}$$

4. APPLICATION

In our application we use the numerical model (see figure 1) of tidally-averaged model flow [De Jong, 1998] with grid size $DX = 1600m$. Because we know the velocities and water depth only in the knots of the grid, we use bilinear interpolation to obtain the velocities and water depth in the arbitrary location. The dispersion coefficient is chosen constant and $D = 5\,m^2/s$.

For this application the reverse system (10) has the following form (we take into account that D is constant)

FIGURE 1. The tidally averaged flow

$$
\begin{aligned}
d\boldsymbol{Y}(s) &= \left(-\boldsymbol{u} - \frac{D}{H}\frac{\partial H}{\partial \boldsymbol{z}}\right) ds + (\sqrt{2D} I_2) d\boldsymbol{W}(s) \\
d\mathcal{Y}(s) &= -\frac{\partial\left(\boldsymbol{u} + \frac{D}{H}\frac{\partial H}{\partial \boldsymbol{z}}\right)}{\partial \boldsymbol{z}^T}\mathcal{Y}(s) ds \\
\boldsymbol{Y}(t) &= \boldsymbol{y},\ \mathcal{Y}(t) = 1,
\end{aligned}
\tag{13}
$$

where $\dfrac{\partial \boldsymbol{F}}{\partial \boldsymbol{x}^T} = \dfrac{\partial \boldsymbol{F}}{\partial x_1} + \dfrac{\partial \boldsymbol{F}}{\partial x_2}$. To solve this equation we use the Euler scheme with time step $h = 3$ min. For the reverse estimator (11) we use the parabolic kernel function

$$
K(\boldsymbol{u}) = \frac{2}{\pi}(1 - \boldsymbol{u}^T\boldsymbol{u}) 1_{\boldsymbol{u}^T\boldsymbol{u} \le 1}, \quad \boldsymbol{u} \in \mathbb{R}^2
$$

and the bandwidth δ

$$
\delta = CN^{-\frac{1}{6}}, \quad C = \left(\frac{1}{N-1}\sum_{n=1}^{N} \|\overline{\boldsymbol{Y}}^{(n)}_{t,\boldsymbol{y}} - \frac{1}{N}\sum_{n=1}^{N} \overline{\boldsymbol{Y}}^{(n)}_{t,\boldsymbol{y}}\|^2\right)^{\frac{1}{2}} - \tag{14}
$$

the standard deviation of the sample $\left\{\overline{Y}^{(m)}\right\}_{m=1,\ldots,M}$.

The figure 2 represents the risk maps for the location $\boldsymbol{y} = (70, 130)$ for 10 days (figure 2 (a),(b)), 15 days (figure 2 (c),(d)) and 20 days (figure 2 (e),(f)). They have been constructed using $N = 10^5$ particles.

These maps give us an idea which location of release may be dangerous for the fixed critical location $\boldsymbol{y}$. For instance, let us consider the risk map for 15 days (see figure 3). If the pollutant was released at point $\boldsymbol{x}_1 = (45, 80)$, then the concentration at critical location $\boldsymbol{y}$ after 15 days would be almost 0. It means that the release of the pollutant at $\boldsymbol{x_1}$ will not affect the point $\boldsymbol{y}$. The location $\boldsymbol{x}_2 = (40, 74)$ is not safe, although the release of the pollutant at this location may lead to the concentration less than $m10^{-10}$

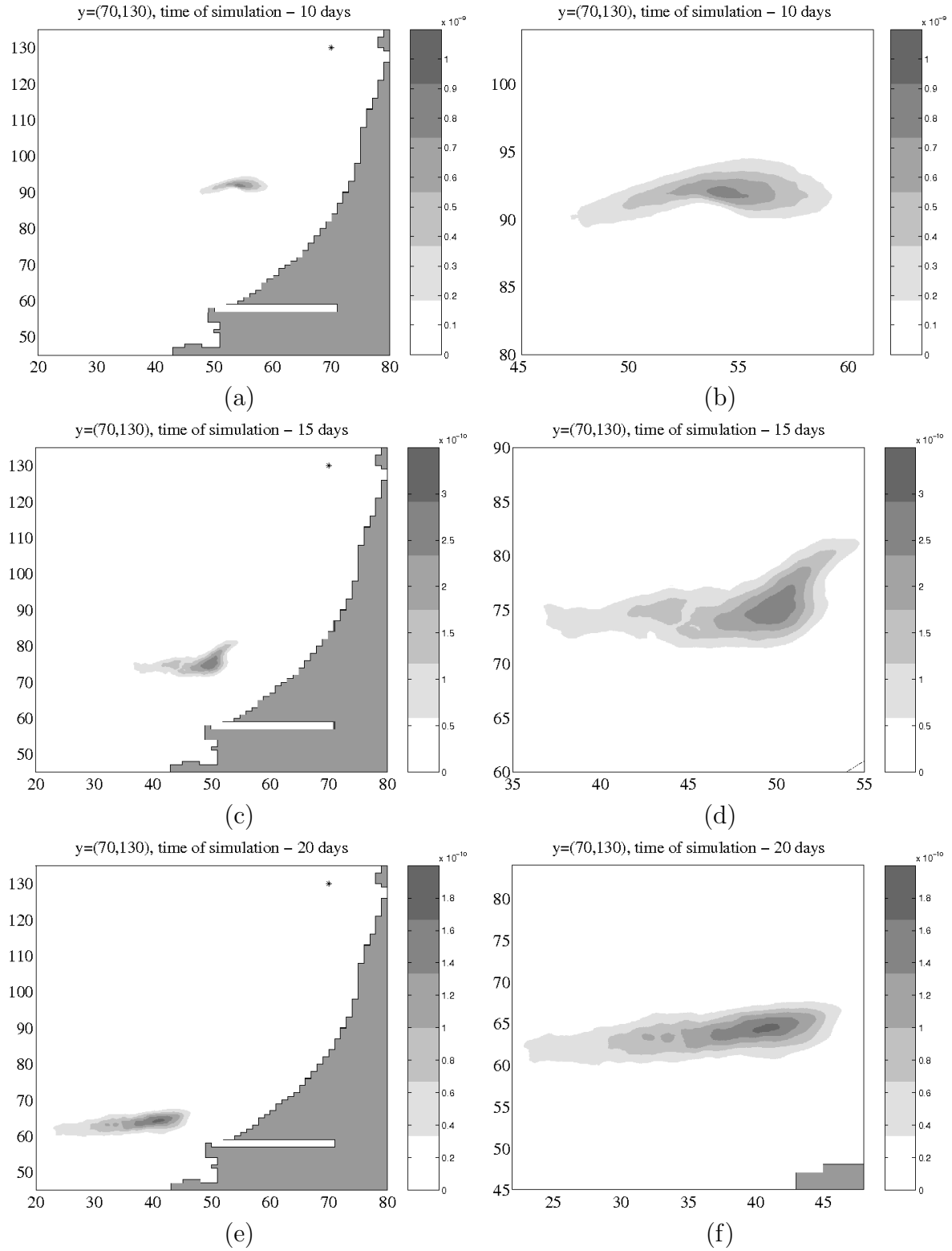

FIGURE 2. The risk map for $y = (70, 130)$ for (a),(b) 10 days, (c),(d) 15 days, (e), (f) 20 days

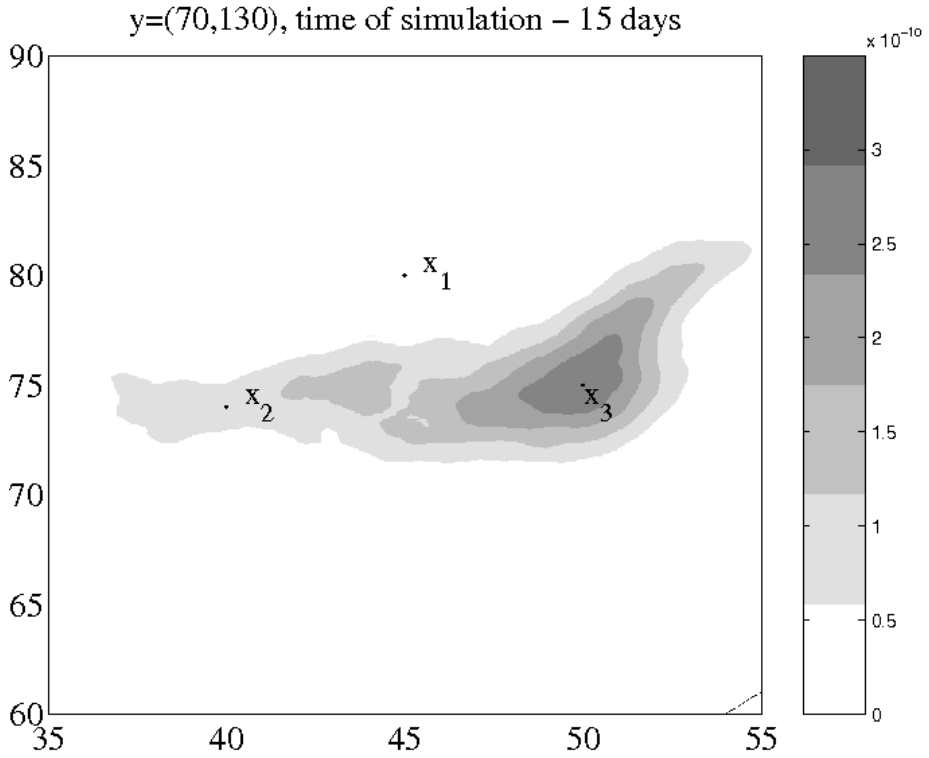

FIGURE 3. The risk map for critical location $\boldsymbol{y} = (70, 130)$ for $T = 15$ days

kg/m^3 (m is mass of initially released pollutant). The release of the pollutant at point $\boldsymbol{x}_3 = (50, 75)$ however would affect the location $\boldsymbol{y}$ very strongly.

In the table 1 one can see the concentration of the pollutant estimated for different location of release $\boldsymbol{x}_1$, $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$. To calculate the concentration the forward (5) and the reverse (11) estimators were applied with different number of particles. Each realization was repeated 30 times to calculate the statistical error of the estimation. From the results in table 1 it is clear that the statistical error has the same order for the both forward and reverse estimators and converges to zero when the number of particles increases.

TABLE 1. The concentration $C(t, \boldsymbol{x}, T, \boldsymbol{y})$ (10^{-10}), kg/m^3

$\boldsymbol{x}$	method	$N = 10^3$	$N = 10^4$	$N = 10^5$
$\boldsymbol{x}_1$	FE	0.003 ± 0.011	0.004 ± 0.005	0.003 ± 0.003
	RE	0.019 ± 0.068	0.005 ± 0.002	0.003 ± 0.001
$\boldsymbol{x}_2$	FE	1.025 ± 0.172	0.958 ± 0.095	0.926 ± 0.046
	RE	0.893 ± 0.247	0.923 ± 0.153	0.904 ± 0.060
$\boldsymbol{x}_3$	FE	2.878 ± 0.295	2.870 ± 0.109	2.897 ± 0.072
	RE	2.552 ± 0.320	2.772 ± 0.120	2.791 ± 0.062

5. CONCLUSION

In this paper the reverse-time diffusion approach is applied to construct the risk maps for certain locations along the Dutch coastline. This method is based on the reverse-time system that can be derived from the original one and is more efficient than the classical forward approach. It is clear that the reverse time approach reduces CPU time orders of magnitude. For several initial location of release the concentration is estimated using the forward and reverse-time approach and the results obtained show that the accuracy of the both methods is almost the same.

References

Anderson, 1982. Anderson BDO (1982), Reverse-time diffusion equation models. Stochastic Processes and their Applications 12: 313-326

Arnold, 1974. Arnold L (1974), Stochastic differential equations. Willey, New York London Sydney Toronto

De Jong, 1998. De Jong K (1998), Tidally averaged transport models. Ph.D. dissertation, Shaker Publishing B.V., Maastricht

Elliott and Anderson, 1985. Elliott RJ, Anderson BDO, Reverse time diffusions, Stochastic Processes and their Applications 19: 327-339

Fischer et al., 1979. Fischer HB, List EJ, Koh RCY, Imberger J, Brooks NH (1979), Mixing in inland and coastal waters. Academic Press, New York

Heemink, 1990. Heemink AW (1990), Stochastic modeling of dispersion in shallow water. Stochastic Hydrol. and Hydraul. 4: 161-174

Jazwinski, 1970. Jazwinski AW (1970) Stochastic differential processes and filtering theory. Academic Press, New York

Kloeden and Platen, 1992. Kloeden PE, Platen E (1992), Numerical solution of stochastic differential equations. Springer, Berlin Heidelberg New York

Kurbanmuradov et al., 1992. Kurbanmuradov O, Rannik U, Sabelfeld K, Vesala T (1992), Direct and adjoint Monte Carlo algorithms for the footprint problem, Monte Carlo methods and Applications 5, nr.2: 85-113

Milstein et al., 2004. Milstein GN, Schoenmakers JGM, Spokoiny V (2004), Transition density estimation for stochastic differential equations via forward-reverse representations. Bernoulli 10, nr. 2: 281-312

Milstein and Tretyakov, 2004. Milstein GN, Tretyakov MV (2004), Stochastic numerics for mathematical physics. Springer, Berlin Heidelberg New York

Oksendal, 1985. Oksendal B (1985) Stochastic differential equations. Springer, Berlin Heidelberg New York

Sabelfeld and Shalimova, 2001. Sabelfeld K, Shalimova I (2001), Forward and Backward Lagrangian stochastic models of turbulent transport, Monte Carlo methods and Applications 7, nr.3-4: 369-383

Silverman 1986. Silverman BW (1986), Density estimation for statistics and data analysis. Champan and Hall, London

Singh and Hager, 1996. Singh VP, Hager WH (1996), Environmental hydraulics. Kluwer Academic Press, Dodrecht

Spivakovskaya et. al, 2005. Spivakovskaya D, Heemink AW, Milstein GN, Schoenmakers JGM (2005) Simulation of the transport of particles in coastal waters using forward and reverse time diffusion, Advances in Water Resources, 28: 927-938

Wand and Jones, 1995. Wand MP, Jones MC (1995), Kernel smoothing. Champan and Hall, London